

~~Susan Hanley~~
Susan Hanley

Access DB# 79295

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: My-Chan Team Examiner #: 78933 Date: 11/4/02
Art Unit: 1639 Phone Number 30 5-6999 Serial Number: 09/871,353
Mail Box and Bldg/Room Location: CM1, 8A16 Results Format Preferred (circle): PAPER DISK E-MAIL
603801

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Functionalized Thiophene oligomers + their use as

Inventors (please provide full names): Franco Cipriani; Giuseppe Gigli; Roberto Lingolani; Laura Favaretto; Massimo Zambianchi; Giovanna Sotgiu; Giovanna Barbieri; Gennaro Citra

Earliest Priority Filing Date: 5/31/00

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Mrs. Hanley,

Please perform the following:

- 1) Inventor search
- 2) Search claim 1-13 (attached)
especially keyword "thiophene oligomer"

Point of Contact
Susan Hanley
Technical Info. Specialist
CM1 6B05 Tel: 305-4053

Thanks!

SEARCHED
SERIALIZED
INDEXED
FILED

search history - a separate query display is attached to each answer set

=> d his

(FILE 'HOME' ENTERED AT 07:18:23 ON 20 NOV 2002)

FILE 'HCAPLUS' ENTERED AT 07:18:34 ON 20 NOV 2002

L1 19 S CIPRIANI F?/AU
L2 135 S GIGLI G?/AU
L3 377 S CINGOLANI R?/AU
L4 48 S FAVARETTO L?/AU
L5 59 S ZAMBIANCHI M?/AU
L6 78 S SOTGIU G?/AU
L7 71 S CITRO G?/AU
L8 132 S BARBARELLA G?/AU
E DELL EMILIA/AU
E EMILIA/AU
E DELLEMILIA/AU
L9 734 S L1-8
L10 54 S L9 AND THIOPHENE
L11 30 S L10 AND OLIGOMER?
L12 5 S L11 AND (THIOPHENE OLIGOMER)/TI 5 citations

Inventor search

SELECT RN L12 1-5 selecting Res # of cpds in L12 citations

FILE 'REGISTRY' ENTERED AT 07:23:58 ON 20 NOV 2002

L13 24 S E49-72 24 cpds


FILE 'HCAPLUS' ENTERED AT 07:24:30 ON 20 NOV 2002

L14 4 S L12 AND L13

L15 5 S L12 OR L14 5 citations w/ 24 cpds displayed

FILE 'REGISTRY' ENTERED AT 07:25:45 ON 20 NOV 2002
SAVE L13 TRA353I/A TEMP

FILE 'REGISTRY' ENTERED AT 07:56:41 ON 20 NOV 2002

L16 STR
L17 289013 S 16.145.3/RID 210 = Ring identifier for 

L18 0 S L16 SSS SAM SUB=L17

L19 STR L16

L20 18 S L19 SSS SAM SUB=L17

L21 5115 S L19 SSS FUL SUB=L17 parent search 5,115 cpds having at least 3  joined together

SAVE L21 TEMP TRA353P/A

L22 50 S L16 SSS SAM SUB=L21

L23 2293 S L16 SSS FUL SUB=L21 subset #1 2293 cpds

SAVE L23 TRA353S1/A TEMP

L24 STR L16

L25 1242 S L24 SSS FUL SUB=L23

SAVE L25 TRA353S2/A TEMP

L26 STR L24

L27 1357 S L26 SSS FUL SUB=L23 subset # 2, 1357 cpds


SAVE L27 TEMP TRA353S3/A

L28 476 S L27 AND 3 16.145.3/RID - 3 thiophene rings

L29 166 S L27 AND 4 16.145.3/RID - 4 " " "

L30 104 S L27 AND 5 16.145.3/RID - 5 " " "

L31 746 S L28-30

L32 674 S L31 AND NC=1 NOT ("DIAZO" OR F/ELS) 674 cpds w/ 3-5  rings and the claimed functional group of Cl 4

L33 23948 S 2 16.145.3/RID ← bithiophene

L34 6084 S L33 AND NR=2

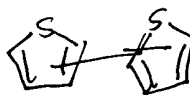
L35 2996 S L33 AND "BITHIOPHENE"

L36 1089 S L35 AND ("HYDROXY" OR "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORM

L37 1089 S L35 AND ("HYDROXY" OR "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORM

Searched by Susan Hanley 305-4053

L33-40 is the search for



TRAN 09/871,353

L38 - searching for
claim 4 functional groups
& 2 ⁵1
"amino" or "thiol"
etc.

L38
L39
L40

662 S L35 AND ("HYDROXY" OR "HYDROXYL" OR "CARBOXYALDEHYDE" OR "FORMY" or
584 S L38 AND NC=1 NC = # components
451 S L39 NOT "AZO" 451 op ds w/ 2 ⁵1

FILE 'HCAPLUS' ENTERED AT 08:40:12 ON 20 NOV 2002

L41
L42
L43
L44
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L58
L59
L60
L61
L62
L63
L64
L65
L66
L67
L68
L69
L70
L71

287 S L32 287 cites for 3-5 thiophene cl 4
455 S L40 455 cites for bi thiophene rings functional groups
15 S L41(L)?CONJUGAT?
14 S L42(L)?CONJUGAT?
26 S L43 OR L44
25 S L45 NOT L15
3042811 S ANTIBOD? OR FLUORESC?(3A)MARKER OR PROTEIN OR DNA OR NUCLEIC
121828 S SPECTROFLUORIMETRY OR CYTOMETRY OR FLUORESCENCE(W)MICROSCO? 0
40 S L41-42 AND L47-48
8 S L49 AND ?CONJUGAT?
7 S L50 NOT L15 7 cites for L40 or L32 oligomers & conjugat.
20 S L46 NOT L51 & claimed uses
18 S L52 NOT PATENT/DT
17 S L53 AND PD<20010530
4 S L54 AND (VISIBLE(3A) (UV OR ULTRAVIOET)) 4 cites
2 S L52 AND PATENT/DT 2 cites
32 S L49 NOT (L50 OR L52)
0 S L57 AND (VISIBLE(3A) (UV OR ULTRAVIOET))
20 S L57 AND ?THIOPHEN?/OBI
20 S L57 AND THIOPHEN?/OBI
12 S L57 AND BITHIOPHEN?/OBI
0 S L57 AND TRITHIOPHEN?/OBI
0 S L57 AND TETRATHIOPHEN?/OBI
0 S L57 AND PENTATHIOPHEN?/OBI
21 S L60-61
2 S L65 AND (?CONJUGAT? OR LINK? OR COVALENT? OR LIGAND). 2 cites
57 S L41-42 AND (VISIBLE(3A) (UV OR ULTRAVIOET))
52 S L67 NOT (L43 OR L45)
15 S L68 AND (?CONJUGAT? OR LINK? OR COVALENT? OR LIGAND)
15 S L69 NOT PATENT/DT
14 S L70 AND PD<20010530 14 citations

FILE 'REGISTRY' ENTERED AT 09:15:59 ON 20 NOV 2002

L72
L73
L74

6 S L32 AND "ISOTHIOCYANATO"
0 S L40 AND "ISOTHIOCYANATO"
0 S "BITHIOPHENE" AND "ISOTHIOCYANATO"

L72-76 looking for
oligothiophene w/
S=C=N group


FILE 'HCAPLUS' ENTERED AT 09:19:51 ON 20 NOV 2002

L75
L76
L77
L78
L79
L80
L81
L82
L83
L84
L85

2 S L72
1 S L75 NOT L15 * 1 cite (applicant) * this specie is disclosed
1392 S OLIGOTHIOPHEN? OR OLIGOMER(3A)?THIOPHEN? only by applicant
2 S L77 AND ISOTHIOCYANAT?
0 S L78 NOT L77
745 S ?THIOPHEN? AND ISOTHIOCYANAT?
264 S ?THIOPHEN?(L) ISOTHIOCYANAT?
1 S L81(L)?CONJUGAT? } appl. stuff
2 S L81 AND ?CONJUGAT?
19 S L81 AND (COVALENT? OR BIND? OR BOUND? OR LINK? OR LIGAND OR ?
5 S L84 AND L47-48 ← not useful

FILE 'STNGUIDE' ENTERED AT 09:26:29 ON 20 NOV 2002

L77-85 - term
searching - didn't
yield anything new
or useful

STR for cpds w/ 3-5 


TRAN 09/871,353

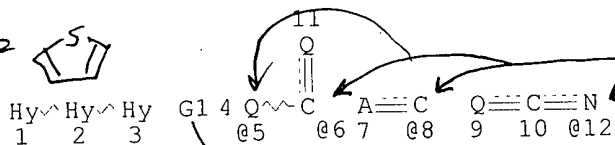
& a functional group

=> d que 141
L16

STR

subset #1

Hy = 



G1 = these functional group
Q = hetero atom
A = non-hydrogen atom

VAR G1=5/6/8/12/NH2/OH/SH/SO3H/SO2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

GGCAT IS MCY UNS AT 2

GGCAT IS MCY UNS AT 3

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E4 C E1 S AT 1

ECOUNT IS E4 C E1 S AT 2

ECOUNT IS E4 C E1 S AT 3

G1 must be present
(connected) to the

Hy - Hy - Hy STR

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12



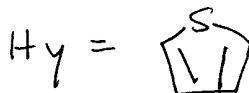
STEREO ATTRIBUTES: NONE

L17 289013 SEA FILE=REGISTRY ABB=ON PLU=ON 16.145.3/RID ← parent set

L19 STR parent STR

Hy¹Hy²Hy³

L1 was searched
against



must be at least 3 thiophenes

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

GGCAT IS MCY UNS AT 2

GGCAT IS MCY UNS AT 3

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E4 C E1 S AT 1

ECOUNT IS E4 C E1 S AT 2

ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

L21 5115 SEA FILE=REGISTRY SUB=L17 SSS FUL L19

L23 2293 SEA FILE=REGISTRY SUB=L21 SSS FUL L16 2293 cpds from subset

L26

STR

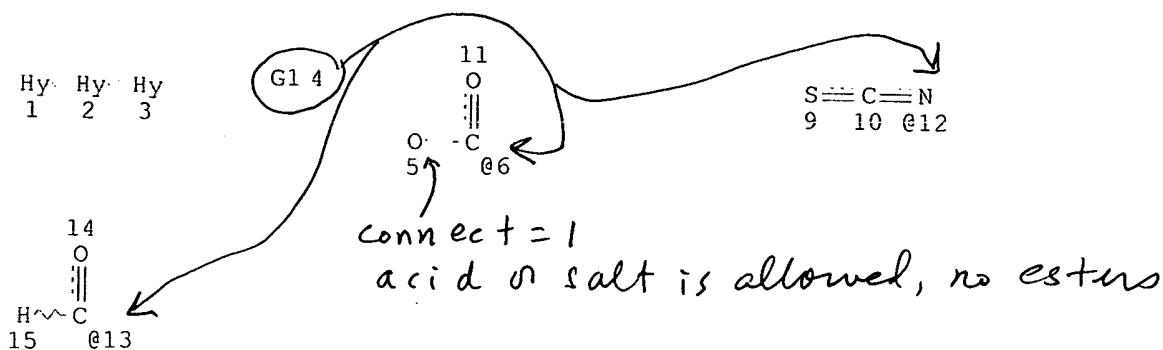
Subset STR #2

STR #1

(over)

subset stk #2

TRAN 09/871,353



VAR G1=OH/SH/NH2/13/6/12 ← claim 4 functional groups

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 5

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

GGCAT IS MCY UNS AT 2

GGCAT IS MCY UNS AT 3

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E4 C E1 S AT 1

ECOUNT IS E4 C E1 S AT 2

ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

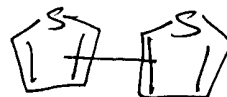
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L27	1357	SEA	FILE=REGISTRY	SUB=L23	SSS	FUL	L26	1357 cpds from subset #
L28	476	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L27	AND 3	16.145.3/RID 3 thiophene
L29	166	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L27	AND 4	16.145.3/RID 4 " "
L30	104	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L27	AND 5	16.145.3/RID 5 " "
L31	746	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	(L28 OR L29 OR L30)		
L32	674	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L31	AND NC=1	NOT ("DIAZO" OR 674 cpds
			F/ELS)					
L41	287	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L32	287 cites for	
							L32 cpds	

search for bi thiophenes

TRAN 09/871,353



Ring ID for

=> d que 142

L33 23948 SEA FILE=REGISTRY ABB=ON PLU=ON 2|16.145.3/RID|

L35 2996 SEA FILE=REGISTRY ABB=ON PLU=ON L33 AND "BITHIOPHENE"

L38 662 SEA FILE=REGISTRY ABB=ON PLU=ON L35 AND ("HYDROXY" OR

"HYDROXYL" OR "CARBOXALDEHYDE" OR "FORMYL" OR "ISOTHIOCYANATO"

OR "THIOL" OR "AMINO" OR "CARBOXYLIC") NOT "ESTER"

} functional groups


L39 584 SEA FILE=REGISTRY ABB=ON PLU=ON L38 AND NC=1

L40 451 SEA FILE=REGISTRY ABB=ON PLU=ON L39 NOT "AZO"

L42 455 SEA FILE=HCAPLUS ABB=ON PLU=ON L40

451 cpds w/

↑
455 cites for L40 cpds

2  is a functional group

Inventor search

TRAN 09/871,353

=> d que 115

L1	19	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	CIPRIANI F?/AU
L2	135	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	GIGLI G?/AU
L3	377	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	CINGOLANI R?/AU
L4	48	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	FAVARETTO L?/AU
L5	59	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	ZAMBIANCHI M?/AU
L6	78	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	SOTGIU G?/AU
L7	71	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	CITRO G?/AU
L8	132	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	BARBARELLA G?/AU
L9	734	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	(L1 OR L2 OR L3 OR L4 OR L5 OR L6 OR L7 OR L8)
L10	54	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L9 AND THIOPHENE
L11	30	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L10 AND OLIGOMER?
L12	5	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L11 AND (THIOPHENE OLIGOMER)/T
L13	24	SEA FILE=REGISTRY	ABB=ON	PLU=ON	(376393-41-8/BI OR 376393-42-9/BI OR 376393-43-0/BI OR 376393-44-1/BI OR 492-97-7/BI OR 111372-97-5/BI OR 111744-23-1/BI OR 113386-74-6/BI OR 116159-99-0/BI OR 118347-89-0/BI OR 127236-47-9/BI OR 127236-48-0/BI OR 127473-73-8/BI OR 127473-74-9/BI OR 127473-75-0/BI OR 139747-07-2/BI OR 139747-08-3/BI OR 14762-74-4/BI OR 201604-95-7/BI OR 201604-98-0/BI OR 25233-34-5/BI OR 376393-45-2/BI OR 5632-29-1/BI OR 67984-20-7/BI)
L14	4	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L12 AND L13
L15	5	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L12 OR L14

5 cita-
tions

searching
Reg# from
L12 cites
-24 cpds

5 cites w/ 24 cpds
displayed

=> d ibib abs hitstr ind 1

L15 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:851250 HCAPLUS

TITLE: Solvent-Free, Microwave-Assisted Synthesis of
Thiophene Oligomers via Suzuki
Coupling

AUTHOR(S): Melucci, Manuela; **Barbarella, Giovanna;**
Sotgiu, Giovanna

CORPORATE SOURCE: Consiglio Nazionale Ricerche (ISOF), Bologna, 40129,
Italy

SOURCE: Journal of Organic Chemistry ACS ASAP
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The purpose of this study was to obtain a rapid, efficient, and environmentally friendly methodol. for the synthesis of highly pure **thiophene oligomers**. The solvent-free, microwave-assisted coupling of thienyl boronic acids and esters with thienyl bromides, using aluminum oxide as the solid support, allowed us to rapidly check the reaction trends on changing times, temp., catalyst, and base and easily optimize the exptl. conditions to obtain the targeted product in fair amts. This procedure offers a novel, general, and very rapid route to the prepn. of sol. **thiophene oligomers**. Thus, for example, quaterthiophene was obtained in 6 min by reaction of 2-bromo-2,2'-bithiophene with bis(pinacolato)diboron (isolated yield 65%), whereas quinquethiophene was obtained in 11 min by reaction of dibromoterthiophene with thienylboronic acid (isolated yield 74%). The synthesis of new chiral 2,2'-bithiophenes is reported. The detailed anal. of the byproducts of some reactions allowed us to elucidate a few aspects of reaction mechanisms. While the use of microwaves proved to be very convenient for the coupling between conventional thienyl moieties, the same was not true for the coupling of thienyl rings to thienyl-S,S-dioxide moieties. Indeed, in this case, the targeted product was obtained in low yields because of the competitive, accelerated, Diels-Alder reaction that affords a variety of condensation products.

CC 35 (Chemistry of Synthetic High Polymers)

=> d ibib abs hitstr ind 2

L15 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:885415 HCAPLUS

DOCUMENT NUMBER: 136:2509

TITLE: Functionalized thiophene oligomers
and their use as fluorescent markersINVENTOR(S): Cipriani, Franco; Gigli, Giuseppe;
Cingolani, Roberto; Favaretto, Laura
; Zambianchi, Massimo; Sotgiu,
Giovanna; Barbarella, Giovanna;
Citro, GennaroPATENT ASSIGNEE(S): Consiglio Nazionale Delle Ricerche, Italy; Istituto
Nazionale Per La Fisica Della Materia; Bio-D S.R.L.
SOURCE: Eur. Pat. Appl., 9 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1160246	A2	20011205	EP 2001-113236	20010530
EP 1160246	A3	20020130		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO

US 2002086437 A1 20020704 US 2001-871353 20010530

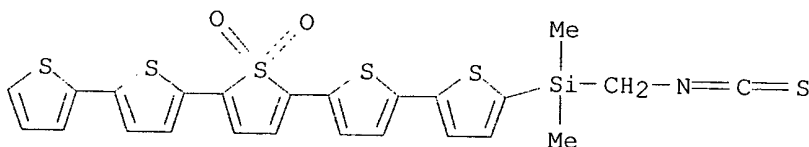
PRIORITY APPLN. INFO.: IT 2000-BA20 A 20000531

AB The invention concerns the synthesis of **thiophene oligomers** and their use as fluorescent markers in anal. techniques. The **oligomers** are excitable in the visible and UV region and have at least one functional group able to form a covalent bond with org. and/or biol. mols., so as not to alter either the fluorescence properties of the **oligomers** or the biol. activity of the bound mols.

IT **376393-44-1D**, conjugates with proteins
RL: ANT (Analyte); ANST (Analytical study)
(functionalized **thiophene oligomers** and use as
fluorescent markers)

RN 376393-44-1 HCAPLUS

CN Silane, (1'',1''-dioxido[2,2':5',2'':5'',2''':5''',2''''-quinguethiophen]-
5-yl)(isothiocyanatomethyl)dimethyl- (9CI) (CA INDEX NAME)

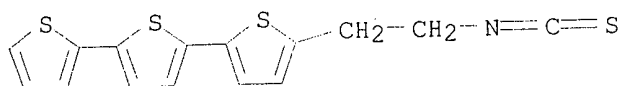


IT **376393-41-8P 376393-42-9P 376393-43-0P**
376393-44-1P

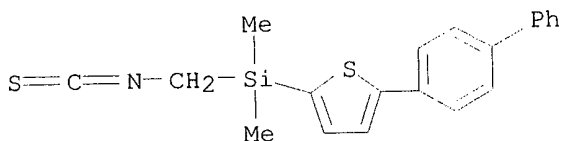
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST
(Analytical study); PREP (Preparation); USES (Uses)
(functionalized **thiophene oligomers** and use as
fluorescent markers)

RN 376393-41-8 HCAPLUS

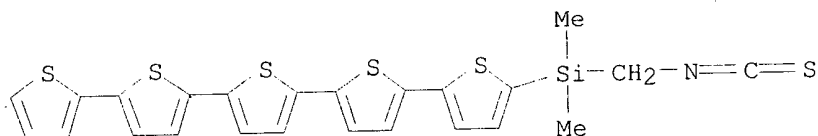
CN 2,2':5',2''-Terthiophene, 5-(2-isothiocyanatoethyl)- (9CI) (CA INDEX NAME)



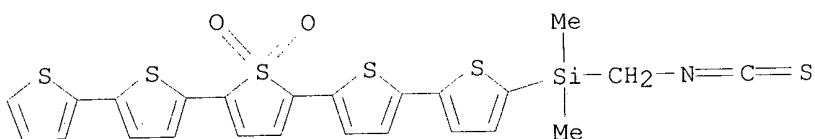
RN 376393-42-9 HCAPLUS
CN Silane, (5-[1,1'-biphenyl]-4-yl-2-thienyl) (isothiocyanatomethyl)dimethyl- (9CI) (CA INDEX NAME)



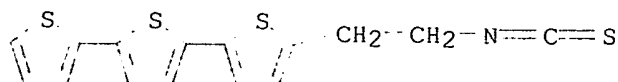
RN 376393-43-0 HCAPLUS
CN Silane, (isothiocyanatomethyl)dimethyl[2,2':5',2'':5'',2''':5''',2''''-quinquethiophen]-5-yl- (9CI) (CA INDEX NAME)



RN 376393-44-1 HCAPLUS
CN Silane, (1'',1'''-dioxido[2,2':5',2'':5'',2''':5''',2''''-quinquethiophen]-5-yl) (isothiocyanatomethyl)dimethyl- (9CI) (CA INDEX NAME)

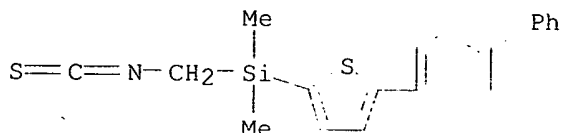


IT 376393-41-8DP, conjugates with proteins 376393-42-9DP,
conjugates with proteins 376393-43-0DP, conjugates with
monoclonal anti-CD8 antibody 376393-45-2DP, conjugates with
albumin
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(functionalized **thiophene oligomers** and use as
fluorescent markers)
RN 376393-41-8 HCAPLUS
CN 2,2':5',2''-Terthiophene, 5-(2-isothiocyanatoethyl)- (9CI) (CA INDEX NAME)



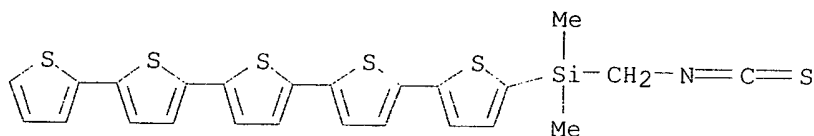
RN 376393-42-9 HCAPLUS

CN Silane, (5-[1,1'-biphenyl]-4-yl-2-thienyl)(isothiocyanatomethyl)dimethyl- (9CI) (CA INDEX NAME)



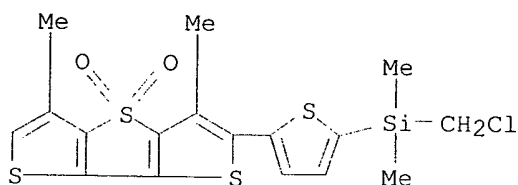
RN 376393-43-0 HCAPLUS

CN Silane, (isothiocyanatomethyl)dimethyl[2,2':5',2'':5'',2''':5''',2''''-quinquethiophen]-5-yl- (9CI) (CA INDEX NAME)



RN 376393-45-2 HCAPLUS

CN Silane, (chloromethyl)[5-(3,5-dimethyl-4,4-dioxidodithieno[3,2-b:2',3'-d]thien-2-yl)-2-thienyl]dimethyl- (9CI) (CA INDEX NAME)



IC ICM C07D333-20

ICS C07D333-48; C07F007-08; G01N033-53

CC 9-14 (Biochemical Methods)

ST **thiophene oligomer** fluorescence marker protein
isothiocyanate fluorometry biol analysis

IT Proteins

RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
(conjugates with synthesized **thiophene oligomers**;
functionalized **thiophene oligomers** and use as
fluorescent markers)

IT Cytometry

(flow; functionalized **thiophene oligomers** and use
as fluorescent markers)

IT Immunoglobulins

RL: ANT (Analyte); ANST (Analytical study)
(fragments; functionalized **thiophene oligomers** and

use as fluorescent markers)

IT Amide group
 Carbonyl group
 Carboxyl group
 Fluorescence microscopy
 Fluorescent substances
 Fluorometry
 Formyl group
 Functional groups
 Gel electrophoresis
 Pharmaceutical analysis
 Sulfhydryl group
 T cell (lymphocyte)
 UV and visible spectroscopy
 (functionalized **thiophene oligomers** and use as
 fluorescent markers)

IT Hormones, animal, analysis
 Neurotransmitters
 Nucleic acids
 Oligonucleotides
 Proteins
 RL: ANT (Analyte); ANST (Analytical study)
 (functionalized **thiophene oligomers** and use as
 fluorescent markers)

IT Functional groups
 (isothiocyanato group; functionalized **thiophene
 oligomers** and use as fluorescent markers)

IT Antibodies
 RL: ANT (Analyte); ANST (Analytical study)
 (monoclonal, CD8; functionalized **thiophene oligomers**
 and use as fluorescent markers)

IT **376393-44-1D**, conjugates with proteins
 RL: ANT (Analyte); ANST (Analytical study)
 (functionalized **thiophene oligomers** and use as
 fluorescent markers)

IT **376393-41-8P 376393-42-9P 376393-43-0P
 376393-44-1P**
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST
 (Analytical study); PREP (Preparation); USES (Uses)
 (functionalized **thiophene oligomers** and use as
 fluorescent markers)

IT **376393-41-8DP**, conjugates with proteins **376393-42-9DP**,
 conjugates with proteins **376393-43-0DP**, conjugates with
 monoclonal anti-CD8 antibody **376393-45-2DP**, conjugates with
 albumin
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (functionalized **thiophene oligomers** and use as
 fluorescent markers)

=> d ibib abs hitstr ind 3

L15 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:686632 HCAPLUS

DOCUMENT NUMBER: 130:25513

TITLE: Structural and Electrical Characterization of
Processable Bis-Silylated Thiophene
OligomersAUTHOR(S): Barbarella, G.; Ostojia, P.; Maccagnani, P.;
Pudova, Olga; Antolini, L.; Casarini, D.; Bongini, A.
CORPORATE SOURCE: I.Co.C.E.A. L.A.M.E.L., Consiglio Nazionale Ricerche,
Bologna, 40129, ItalySOURCE: Chemistry of Materials (1998), 10(11), 3683-3689
CODEN: CMATEX; ISSN: 0897-4756

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

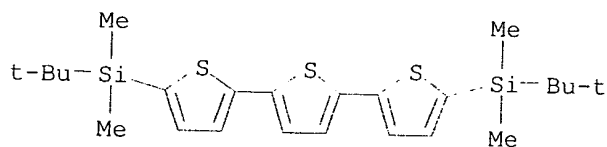
AB A new class of processable, chem. stable, and easily synthesized and purified .alpha.,.omega.-bis(dimethyl-tert-butylsilyl) oligothiophenes is described. Information on the solid-state properties was obtained by single crystal X-ray diffraction and CPMAS NMR spectroscopy. Mol. packing was characterized by a sandwich-type organization, with the mol. planes between adjacent layers along the stacking direction being exactly parallel. Vacuum-evapd. thin films of the tetramer, pentamer, and hexamer displayed field effect transistor activity, with charge mobilities increasing with the substrate deposition temps. in the range 28-80 .degree.C. The best FET performance was achieved with the pentamer which was characterized by an on/off ratio > 103, reproducibility, and a device stability in air of months.

IT 201604-95-7 201604-98-0

RL: PRP (Properties)
(structural and elec. characterization of processable bis-silylated
thiophene oligomers)

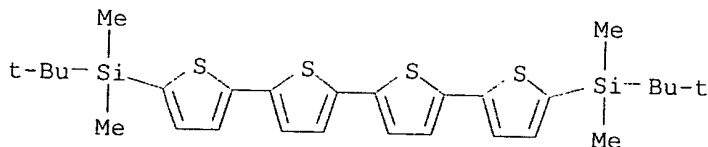
RN 201604-95-7 HCAPLUS

CN Silane, 2,2':5',2''-terthiophene-5,5'''-diylbis[(1,1-dimethylethyl)dimethyl-
(9CI) (CA INDEX NAME)]



RN 201604-98-0 HCAPLUS

CN Silane, 2,2':5',2'':5'',2'''-quaterthiophene-5,5'''-diylbis[(1,1-
dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)]



CC 36-2 (Physical Properties of Synthetic High Polymers)
Section cross-reference(s): 76

ST bis silylated **thiophene oligomer** structure elec
property

IT MAS NMR spectroscopy
(CP; structural and elec. characterization of processable bis-silylated
thiophene oligomers)

IT Polymers, properties
RL: PRP (Properties)
(polythiophenes, **oligomeric**, silane-terminated; structural
and elec. characterization of processable bis-silylated
thiophene oligomers)

IT Crystal structure
Field effect transistors
Polymer chains
(structural and elec. characterization of processable bis-silylated
thiophene oligomers)

IT 201604-95-7 201604-98-0
RL: PRP (Properties)
(structural and elec. characterization of processable bis-silylated
thiophene oligomers)

REFERENCE COUNT: 42

THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr ind 4

L15 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:150890 HCAPLUS

DOCUMENT NUMBER: 116:150890

TITLE: Conformation and optical absorption properties of
thiophene oligomers: carbon-13 NMR,
UV, and MMP2 calculations of di- and
tetramethylquaterthiophenesAUTHOR(S): Barbarella, Giovanna; Bongini, Alessandro;
Zambianchi, MassimoCORPORATE SOURCE: Inst. Composti Carbonio Contenenti Eteroatomi Loro
Appl., Ozzano Emilia, I-40066, ItalySOURCE: Advanced Materials (Weinheim, Germany) (1991), 3(10),
494-6

CODEN: ADVMEW; ISSN: 0935-9648

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 13C NMR and UV data, together with MMP2 calcns., indicate that the degree
of planarity of quaterthiophenes in soln. is given by the cis junctions
between adjacent rings and that only the presence of 2 Me in the 3,3'
positions of a bithiophene subsystem freezes the conformation in the anti
orientation, leading to the system being markedly non-planar.

IT 492-97-7, 2,2'-Bithiophene 67984-20-7

111372-97-5 113386-74-6 116159-99-0

118347-89-0 127236-48-0 139747-08-3

RL: PRP (Properties)

(carbon-13 NMR and UV of, conjugation and)

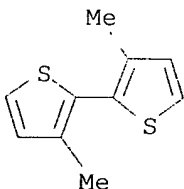
RN 492-97-7 HCAPLUS

CN 2,2'-Bithiophene (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



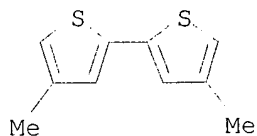
RN 67984-20-7 HCAPLUS

CN 2,2'-Bithiophene, 3,3'-dimethyl- (6CI, 9CI) (CA INDEX NAME)

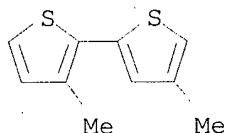


RN 111372-97-5 HCAPLUS

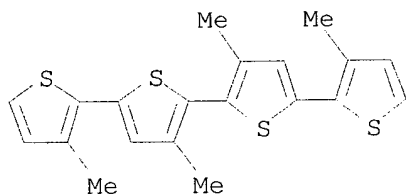
CN 2,2'-Bithiophene, 4,4'-dimethyl- (9CI) (CA INDEX NAME)



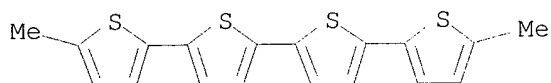
RN 113386-74-6 HCAPLUS
CN 2,2'-Bithiophene, 3,4'-dimethyl- (9CI) (CA INDEX NAME)



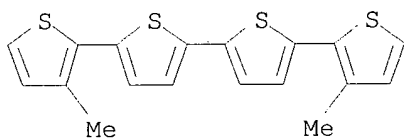
RN 116159-99-0 HCAPLUS
CN 2,2':5',2'':5'''-Quaterthiophene, 3,3'',3''',4'-tetramethyl- (9CI)
(CA INDEX NAME)



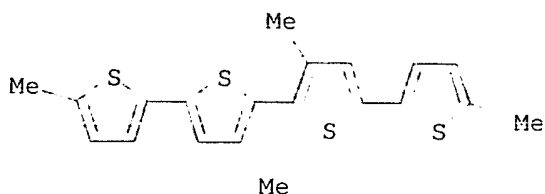
RN 118347-89-0 HCAPLUS
CN 2,2':5',2'':5'''-Quaterthiophene, 5,5'''-dimethyl- (9CI) (CA INDEX NAME)



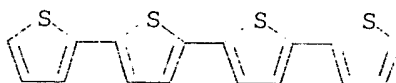
RN 127236-48-0 HCAPLUS
CN 2,2':5',2'':5'''-Quaterthiophene, 3,3'''-dimethyl- (9CI) (CA INDEX NAME)



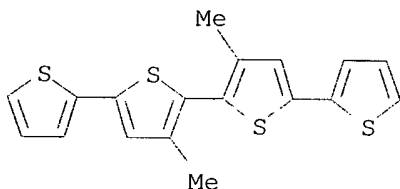
RN 139747-08-3 HCAPLUS
CN 2,2':5',2'':5'''-Quaterthiophene, 3'',4',5,5'''-tetramethyl- (9CI)
(CA INDEX NAME)



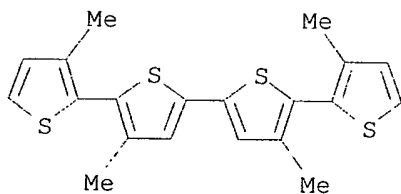
IT 5632-29-1, Quaterthiophene 127236-47-9
 139747-07-2
 RL: PRP (Properties)
 (carbon-13 NMR in UV, mol. mechanics, and conformation of, conjugation and)
 RN 5632-29-1 HCAPLUS
 CN 2,2':5',2'':5'',2'''-Quaterthiophene (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 127236-47-9 HCAPLUS
 CN 2,2':5',2'':5'',2'''-Quaterthiophene, 3'',4'-dimethyl- (9CI) (CA INDEX NAME)



RN 139747-07-2 HCAPLUS
 CN 2,2':5',2'':5'',2'''-Quaterthiophene, 3,3',3'',4''-tetramethyl- (9CI)
 (CA INDEX NAME)



IT 14762-74-4
 RL: PRP (Properties)
 (nuclear magnetic resonance, of quaterthiophene and related compds., carbon-13)
 RN 14762-74-4 HCAPLUS
 CN Carbon, isotope of mass 13 (8CI, 9CI) (CA INDEX NAME)

13C

- CC 22-3 (Physical Organic Chemistry)
 ST UV methylquaterthiophene; carbon NMR methylquaterthiophene; conformation
 methylquaterthiophene mol mechanism
 IT Methyl group
 (effect of, on conformation of quaterthiophene and related compds.)
 IT Conjugation
 Hyperconjugation
 (in quaterthiophene and related compds.)
 IT Conformation and Conformers
 (of quaterthiophene and related compds.)
 IT Nuclear magnetic resonance
 (of quaterthiophene and related compds., carbon-13)
 IT Molecular mechanics
 (of quaterthiophene and related compds., conformation and)
 IT Ultraviolet and visible spectra
 (of quaterthiophene and related compds., conjugation and)
 IT 492-97-7, 2,2'-Bithiophene 67984-20-7
 111372-97-5 113386-74-6 116159-99-0
 118347-89-0 127236-48-0 139747-08-3
 RL: PRP (Properties)
 (carbon-13 NMR and UV of, conjugation and)
 IT 5632-29-1, Quaterthiophene 127236-47-9
 139747-07-2
 RL: PRP (Properties)
 (carbon-13 NMR in UV, mol. mechanics, and conformation of, conjugation
 and)
 IT 14762-74-4
 RL: PRP (Properties)
 (nuclear magnetic resonance, of quaterthiophene and related compds.,
 carbon-13)

=> d ibib abs hitstr ind 5

L15 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1990:460286 HCAPLUS

DOCUMENT NUMBER: 113:60286

TITLE: Determination of the electronic structure of
thiophene oligomers and
extrapolation to polythiopheneAUTHOR(S): Jones, Derek; Guerra, Maurizio; Favaretto,
Laura; Modelli, Alberto; Fabrizio, Monica;
Distefano, Giuseppe

CORPORATE SOURCE: ICoCEA, Cons. Naz. Ric., Ozzano Emilia, 40064, Italy

SOURCE: Journal of Physical Chemistry (1990), 94(15), 5761-6
CODEN: JPCHAX; ISSN: 0022-3654

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Ionization energies, attachment energies, and electrochem. redn. potentials of **thiophene oligomers** (d.p. .ltoreq.5) were detd. exptl. (UV photoelectron and electron transmission spectroscopies and cyclic voltammetry) and theor. (ionization and attachment energies by MINDO/3). The geometrical parameters of the most stable conformation of 2,2'-bithienyl were computed at the ab initio STO-3G level with complete relaxation. A short extrapolation of the energy data to the polymer provided accurate and reliable values for important properties of polythiophene in the gas phase, namely: ionization energy 6.9 eV, valence bandwidth 3.2 eV, electron affinity 0.9.apprx.1.1 eV, HOMO-LUMO energy gap 5.9 eV, and .lambda.max 2.7 eV.

IT 25233-34-5, **Thiophene** homopolymer

RL: PRP (Properties)

(electronic structure of, electronic structure of **oligomers**
in relation to)

RN 25233-34-5 HCAPLUS

CN Thiophene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 110-02-1

CMF C4 H4 S

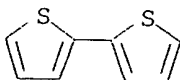
IT 492-97-7, 2,2'-Bithiophene 111744-23-1, Terthiophene
127473-73-8 127473-74-9 127473-75-0

RL: PRP (Properties)

(electronic structure of, polythiophene electronic structure in
relation to)

RN 492-97-7 HCAPLUS

CN 2,2'-Bithiophene (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 111744-23-1 HCAPLUS
 CN Terthiophene (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 127473-73-8 HCAPLUS
 CN Thiophene, tetramer (9CI) (CA INDEX NAME)

CM 1

CRN 110-02-1
 CMF C4 H4 S



RN 127473-74-9 HCAPLUS
 CN Thiophene, pentamer (9CI) (CA INDEX NAME)

CM 1

CRN 110-02-1
 CMF C4 H4 S



RN 127473-75-0 HCAPLUS
 CN Thiophene, hexamer (9CI) (CA INDEX NAME)

CM 1

CRN 110-02-1
 CMF C4 H4 S



CC 36-5 (Physical Properties of Synthetic High Polymers)
 ST **thiophene oligomer** polymer electronic structure;
 ionization energy **thiophene oligomer** polymer;
 attachment energy **thiophene oligomer** polymer;
 electrochem redn potential **thiophene oligomer**;
 conformation **thiophene oligomer** polymer; valence
 bandwidth **thiophene oligomer**; electron affinity
thiophene oligomer polymer; energy gap **thiophene
 oligomer** polymer
 IT Chains, chemical
 (conformation of, in **thiophene oligomers**)
 IT Ionization potential and energy
 (of **thiophene oligomers**, electronic structure of
 polythiophene in relation to)

- IT Electron affinity
 (of thiophene oligomers, electronic structure of
 thiophene polymers in relation to)
- IT Molecular orbital
 (MINDO/3, of thiophene oligomers)
- IT Molecular orbital
 (frontier, of thiophene oligomers)
- IT Energy level, band structure
 (gap, of thiophene oligomers, polythiophene
 electronic structure in relation to)
- IT Electric potential
 (redn., of thiophene oligomers, electronic
 structure of polythiophene in relation to)
- IT Energy level, band structure
 (valence, of thiophene oligomers, electronic
 structure of polythiophene in relation to)
- IT 25233-34-5, Thiophene homopolymer
 RL: PRP (Properties)
 (electronic structure of, electronic structure of oligomers
 in relation to)
- IT 492-97-7, 2,2'-Bithiophene 111744-23-1, Terthiophene
 127473-73-8 127473-74-9 127473-75-0
 RL: PRP (Properties)
 (electronic structure of, polythiophene electronic structure in
 relation to)

=> d que 151

L1 19 SEA FILE=HCAPLUS ABB=ON PLU=ON CIPRIANI F?/AU
 L2 135 SEA FILE=HCAPLUS ABB=ON PLU=ON GIGLI G?/AU
 L3 377 SEA FILE=HCAPLUS ABB=ON PLU=ON CINGOLANI R?/AU
 L4 48 SEA FILE=HCAPLUS ABB=ON PLU=ON FAVARETTO L?/AU
 L5 59 SEA FILE=HCAPLUS ABB=ON PLU=ON ZAMBIANCHI M?/AU
 L6 78 SEA FILE=HCAPLUS ABB=ON PLU=ON SOTGIU G?/AU
 L7 71 SEA FILE=HCAPLUS ABB=ON PLU=ON CITRO G?/AU
 L8 132 SEA FILE=HCAPLUS ABB=ON PLU=ON BARBARELLA G?/AU
 L9 734 SEA FILE=HCAPLUS ABB=ON PLU=ON (L1 OR L2 OR L3 OR L4 OR L5
 OR L6 OR L7 OR L8)
 L10 54 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 AND THIOPHENE
 L11 30 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 AND OLIGOMER?
 L12 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L11 AND (THIOPHENE OLIGOMER)/T
 I
 L13 24 SEA FILE=REGISTRY ABB=ON PLU=ON (376393-41-8/BI OR 376393-42-
 9/BI OR 376393-43-0/BI OR 376393-44-1/BI OR 492-97-7/BI OR
 111372-97-5/BI OR 111744-23-1/BI OR 113386-74-6/BI OR 116159-99
 -0/BI OR 118347-89-0/BI OR 127236-47-9/BI OR 127236-48-0/BI OR
 127473-73-8/BI OR 127473-74-9/BI OR 127473-75-0/BI OR 139747-07
 -2/BI OR 139747-08-3/BI OR 14762-74-4/BI OR 201604-95-7/BI OR
 201604-98-0/BI OR 25233-34-5/BI OR 376393-45-2/BI OR 5632-29-1/
 BI OR 67984-20-7/BI)
 L14 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L12 AND L13
 L15 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L12 OR L14 5 cites from applicants
 L16 STR

inv.
search1st subset STR

11

Q

Hy¹Hy²Hy³ G1 4 Q⁵C⁶ A⁷C⁸ Q⁹C¹⁰N¹²
 1 2 3 @5 @6 7 @8 9 10 @12

VAR G1=5/6/8/12/NH2/OH/SH/SO3H/SO2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

GGCAT IS MCY UNS AT 2

GGCAT IS MCY UNS AT 3

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E4 C E1 S AT 1

ECOUNT IS E4 C E1 S AT 2

ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L17 289013 SEA FILE=REGISTRY ABB=ON PLU=ON 16.145.3/RID

L19 STR

parent search

Hy¹Hy²Hy³
 1 2 3

Hy =



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

GGCAT IS MCY UNS AT 2

the STR search to
 obtain L32 answer set
 (cpds w/ 3-5 [5]) + term
 search to get L40 (bi thiophene,
 etc.)

TRAN 09/871,353

GGCAT IS MCY UNS AT 3
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E1 S AT 1
ECOUNT IS E4 C E1 S AT 2
ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

L21 5115 SEA FILE=REGISTRY SUB=L17 SSS FUL L19
L23 2293 SEA FILE=REGISTRY SUB=L21 SSS FUL L16
L26 STR *2nd subset STR*

Hy Hy Hy G1 4
1 2 3
O
||
O-C
5 @6
S=C=N
9 10 @12

14
O
||
H-C
15 @13

VAR G1=OH/SH/NH2/13/6/12

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 5
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY UNS AT 1
GGCAT IS MCY UNS AT 2
GGCAT IS MCY UNS AT 3
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E1 S AT 1
ECOUNT IS E4 C E1 S AT 2
ECOUNT IS E4 C E1 S AT 3


GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L27 1357 SEA FILE=REGISTRY SUB=L23 SSS FUL L26
L28 476 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 3 16.145.3/RID
L29 166 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 4 16.145.3/RID
L30 104 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 5 16.145.3/RID
L31 746 SEA FILE=REGISTRY ABB=ON PLU=ON (L28 OR L29 OR L30)
L32 674 SEA FILE=REGISTRY ABB=ON PLU=ON L31 AND NC=1 NOT ("DIAZO" OR F/ELS) *674 cpds*
L33 23948 SEA FILE=REGISTRY ABB=ON PLU=ON 2 16.145.3/RID
L35 2996 SEA FILE=REGISTRY ABB=ON PLU=ON L33 AND "BITHIOPHENE" *3-5*
L38 662 SEA FILE=REGISTRY ABB=ON PLU=ON L35 AND ("HYDROXY" OR "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORMYL" OR "ISOTHIOCYANATO" OR "THIOL" OR "AMINO" OR "CARBOXYLIC") NOT "ESTER" *5 rings*
L39 584 SEA FILE=REGISTRY ABB=ON PLU=ON L38 AND NC=1
L40 451 SEA FILE=REGISTRY ABB=ON PLU=ON L39 NOT "AZO" *451 cpds w/ 2*
L41 287 SEA FILE=HCAPLUS ABB=ON PLU=ON L32 *287 cites for L32 cpds*

Searched by Susan Hanley 305-4053

TRAN 09/871,353

L42 455 SEA FILE=HCAPLUS ABB=ON PLU=ON L40 455 cites for 2 
L47 3042811 SEA FILE=HCAPLUS ABB=ON PLU=ON ANTIBOD? OR FLUORESC?(3A)MARKE
R OR PROTEIN OR DNA OR NUCLEIC OR OLIGONUC? OR HORMON? OR DRUG
OR MEDICINE OR NEUROTRANSMITTER
L48 121828 SEA FILE=HCAPLUS ABB=ON PLU=ON SPECTROFLUORIMETRY OR
CYTOMETRY OR FLUORESCENCE(W)MICROSCO? OR GEL ELECTROPHOR?
L49 40 SEA FILE=HCAPLUS ABB=ON PLU=ON (L41 OR L42) AND (L47 OR L48)
L50 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L49 AND ?CONJUGAT?
L51 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L50 NOT L15 7 cites

subtracting out
applicant's work

=> d ibib abs hitstr 1

L51 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:792698 HCAPLUS

DOCUMENT NUMBER: 136:66480

TITLE: Oligothiophene isothiocyanates as a new class of
fluorescent markers for biopolymersAUTHOR(S): Barbarella, Giovanna; Zambianchi, Massimo; Pudova,
Olga; Paladini, Vanessa; Ventola, Alfredo; Cipriani,
Francesco; Gigli, Giuseppe; Cingolani, Roberto; Citro,
GennaroCORPORATE SOURCE: Consiglio Nazionale Ricerche, I.Co.C.E.A, Bologna,
40129, ItalySOURCE: Journal of the American Chemical Society (2001),
123(47), 11600-11607

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The regioselective synthesis of fluorescent oligothiophene isothiocyanates is described. The isothiocyanates were reacted with bovine serum albumin (BSA) following std. procedures and the optical properties of the oligothiophene-BSA **conjugates** were analyzed as a function of oligomer concn., time, and irradiation power. The oligothiophene-BSA **conjugates** were chem. very stable and their photoluminescence characteristics persisted unaltered for several months. Photoluminescence data relative to the **conjugate** of an oligothiophene-S,S-dioxide isothiocyanate with monoclonal anti-CD8 **antibody** are reported. No fluorescence quenching was observed following the binding of the isothiocyanate to the **antibody** and the **conjugate** displayed high chem. stability and photostability.

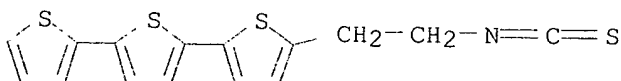
IT 376393-41-8DP, reaction **conjugated** with bovine serum albumin 385369-25-5DP, reaction **conjugated** with bovine serum albumin 385369-31-3DP, reaction **conjugated** with bovine serum albumin 385369-34-6DP, reaction **conjugated** with CD8 **antibody**

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)

(oligothiophene isothiocyanates as a new class of **fluorescent markers** for biopolymers)

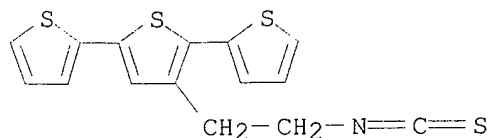
RN 376393-41-8 HCAPLUS

CN 2,2':5',2''-Terthiophene, 5-(2-isothiocyanatoethyl)- (9CI) (CA INDEX NAME)



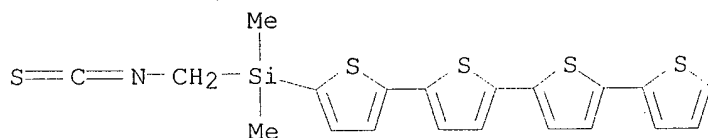
RN 385369-25-5 HCAPLUS

CN 2,2':5',2''-Terthiophene, 3'-(2-isothiocyanatoethyl)- (9CI) (CA INDEX NAME)



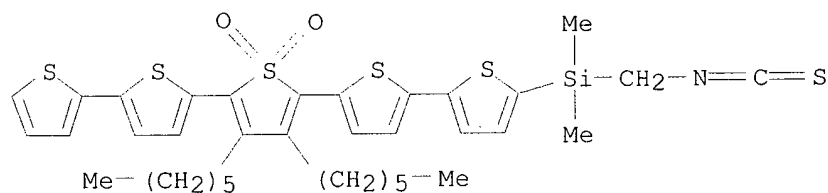
RN 385369-31-3 HCAPLUS

CN Silane, (isothiocyanatomethyl)dimethyl[2,2':5',2'':5'''-quaterthiophen]-5-yl- (9CI) (CA INDEX NAME)



RN 385369-34-6 HCAPLUS

CN Silane, (3'',4''-dihexyl-1'',1''-dioxido[2,2',5':2'':5'''-quaterthiophen]-5-yl)(isothiocyanatomethyl)dimethyl- (9CI) (CA INDEX NAME)



IT 273400-09-2P, [2,2':5',2'':Terthiophene]-3'-ethanol

385369-23-3P, [2,2':5',2'':Terthiophene]-3'-ethanamine

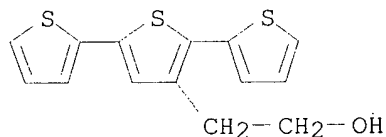
385369-24-4P, [2,2':5',2'':Terthiophene]-5-ethanamine

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(oligothiophene isothiocyanates as a new class of **fluorescent markers** for biopolymers)

RN 273400-09-2 HCAPLUS

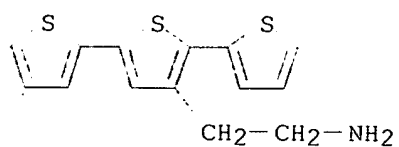
CN [2,2':5',2'':Terthiophene]-3'-ethanol (9CI) (CA INDEX NAME)



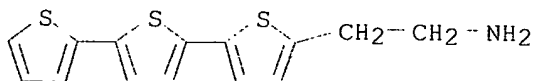
RN 385369-23-3 HCAPLUS

CN [2,2':5',2'':Terthiophene]-3'-ethanamine (9CI) (CA INDEX NAME)

TRAN 09/871,353



RN 385369-24-4 HCAPLUS
CN [2,2':5',2''-Terthiophene]-5-ethanamine (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 2

L51 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:699243 HCAPLUS

DOCUMENT NUMBER: 136:32334

TITLE: Direct DNA hybridization detection based on the **oligonucleotide**-functionalized conductive polymer

AUTHOR(S): Lee, Tae-Young; Shim, Yoon-Bo

CORPORATE SOURCE: Department of Chemistry, Pusan National University, Keumjeong-ku Pusan, 609-735, S. Korea

SOURCE: Analytical Chemistry (2001), 73(22), 5629-5632
CODEN: ANCHAM; ISSN: 0003-2700

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Electrochem. methods for **DNA** hybridization detection have many advantages that are very fast to detect hybridization and can be directly applied for a portable **DNA** sensor. In this paper, an electrochem. method to directly detect **DNA** hybridization was developed on the basis of a new conductive polymer, which was polymd. on the glassy carbon electrode with a terthiophene monomer having a carboxyl group (3'-carboxyl-5,2',5',2''-terthiophene). The ss-**DNA** probe was made by chem. bonding an amine-linked C6 alkyl group to the 5' terminus of **oligonucleotide** (19-mer). The probe moiety was immobilized on the polymer through covalent bonding with a catalyst, 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide. A difference in admittance was obsd. before and after hybridization as a result of the redn. of the resistance after hybridization. The highest difference in admittance was obsd. around 1 kHz before and after hybridization. Hybridization amts. of end two-base and center one-base mismatched sequences were obtained only in a 14.3% response when compared to that for the complementary matched sequence.

IT 380630-96-6P

RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(direct **DNA** hybridization detection based on **oligonucleotide**-functionalized conductive polymer)

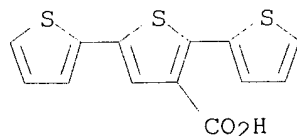
RN 380630-96-6 HCAPLUS

CN [2,2':5',2''-Terthiophene]-3'-carboxylic acid, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 380630-95-5

CMF C13 H8 O2 S3



REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ind 2

L51 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2002 ACS
 CC 3-1 (Biochemical Genetics)
 Section cross-reference(s): 9
 ST DNA hybridization detection **oligonucleotide** conductive
 polymer probe
 IT Nucleic acid hybridization
 (DNA-DNA; direct DNA hybridization
 detection based on **oligonucleotide**-functionalized conductive
 polymer)
 IT Oligonucleotides
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST
 (Analytical study); PREP (Preparation); USES (Uses)
 (amine-linked C6 alkyl group **conjugates**; direct DNA
 hybridization detection based on **oligonucleotide**
 -functionalized conductive polymer)
 IT Conducting polymers
 (direct DNA hybridization detection based on
oligonucleotide-functionalized conductive polymer)
 IT Electrodes
 (glassy carbon, polymn. on; direct DNA hybridization
 detection based on **oligonucleotide**-functionalized conductive
 polymer)
 IT Electric conductivity
 (measurement, and hybridization detection; direct DNA
 hybridization detection based on **oligonucleotide**
 -functionalized conductive polymer)
 IT Probes (**nucleic acid**)
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST
 (Analytical study); PREP (Preparation); USES (Uses)
 (**oligonucleotide** bonding amine-linked C6 alkyl group; direct
 DNA hybridization detection based on **oligonucleotide**
 -functionalized conductive polymer)
 IT Electric resistance
 (redn. of, after hybridization; direct DNA hybridization
 detection based on **oligonucleotide**-functionalized conductive
 polymer)
 IT 1892-57-5, 1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst; direct DNA hybridization detection based on
oligonucleotide-functionalized conductive polymer)
 IT 380630-96-6P
 RL: DEV (Device component use); SPN (Synthetic preparation); PREP
 (Preparation); USES (Uses)
 (direct DNA hybridization detection based on
oligonucleotide-functionalized conductive polymer)

=> d ibib abs hitstr 3

L51 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:41752 HCAPLUS

DOCUMENT NUMBER: 132:194595

TITLE: Novel nucleoside analogues with fluorophores replacing the DNA base

AUTHOR(S): Strassler, Christoph; Davis, Newton E.; Kool, Eric T.

CORPORATE SOURCE: Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA

SOURCE: Helvetica Chimica Acta (1999), 82(12), 2160-2171

CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We describe the prepn. and fluorescence properties of a set of new nucleosides in which a known hydrocarbon or oligothiophene fluorophore replaces the DNA base at C(1) of the deoxyribose moiety. These compds. are potentially useful as probes in the study of the structure and dynamics of nucleic acids and their complexes with proteins. In addn., they may find use as fluorescent labels for nucleic-acid-based biomedical diagnostics methods. The fluorophores conjugated to deoxyribose at C(1) in the .alpha.-D-form include terphenyl, stilbene, terthiophene, benzoterthiophene, and pyrene. Also included is a non-fluorescent spacer in which cyclohexene replaces the DNA base. The nucleosides are derived from brominated fluorophore precursors and Hoffer's 2-deoxy-3,5-di-O-(p-toluoyl)-D-ribofuranosyl chloride. The emission maxima of the free nucleosides range from 345 to 536 nm. Also described are the 5'-(dimethoxytrityl) 3'-O-phosphoramidite derivs. suitable for incorporation into oligonucleotides by automated synthesizers.

IT 259801-06-4P 259801-07-5P

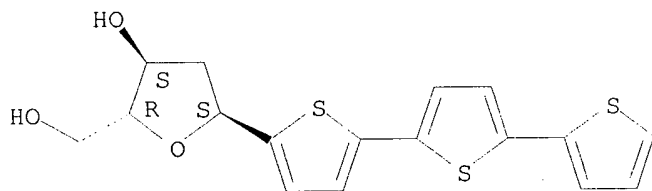
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of novel nucleoside analogs with fluorophores replacing the DNA base)

RN 259801-06-4 HCAPLUS

CN D-erythro-Pentitol, 1,4-anhydro-2-deoxy-1-C-[2,2':5',2''-terthiophen]-5-yl-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

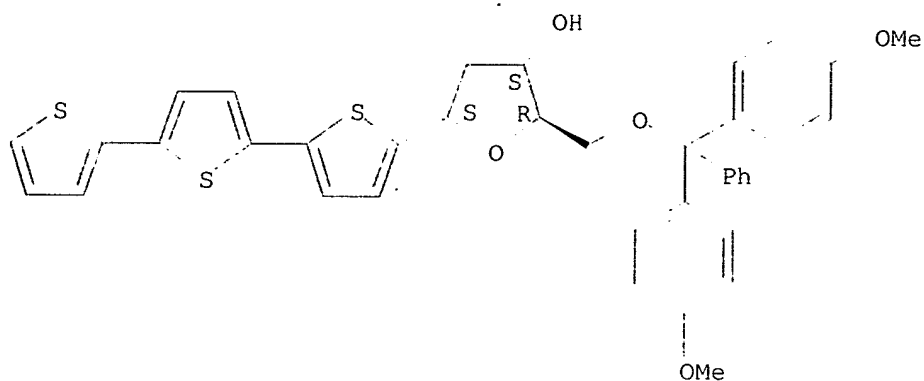


RN 259801-07-5 HCAPLUS

CN D-erythro-Pentitol, 1,4-anhydro-5-O-[bis(4-methoxyphenyl)phenylmethyl]-2-deoxy-1-C-[2,2':5',2''-terthiophen]-5-yl-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

TRAN 09/871,353



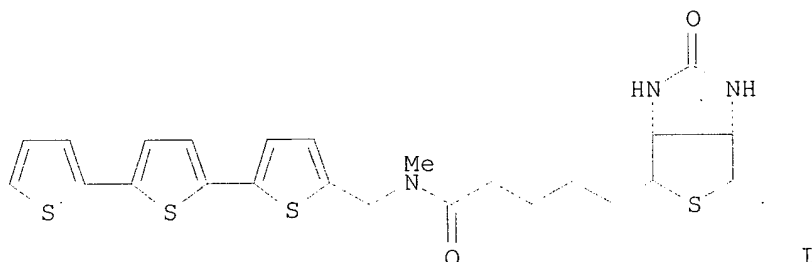
REFERENCE COUNT:

39

THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 4

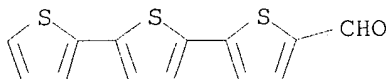
L51 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1996:528314 HCAPLUS
 DOCUMENT NUMBER: 125:300730
 TITLE: A new synthetic route to 2,2':5',2''-terthiophene-5-derivatives to **conjugate** with **proteins** and monoclonal **antibodies**
 AUTHOR(S): Cosimelli, Barbara; Neri, Dario; Roncucci, Gabrio
 CORPORATE SOURCE: Molteni Farmaceutici, Florence, Italy
 SOURCE: Tetrahedron (1996), 52(34), 11281-11290
 CODEN: TETRAB; ISSN: 0040-4020
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB A no. of terthiophene derivs. which can be linked to **proteins** or other carrier mols. by using different functional groups were synthesized and characterized. The **conjugation** of some of these compds. to carrier **proteins** and **antibodies** was described. An example compd. is the N-[(terthienyl)methyl]biotinpentanamide **conjugate** I. The possible applications of I as photosensitizer were discussed (no data).

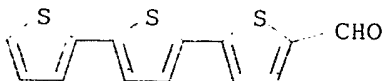
IT **7342-41-8DP**, [2,2':5',2''-Terthiophene]-5-carboxaldehyde, **conjugates** with **proteins** or **antibodies**
 RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
 (prepn. of terthiophene **conjugates** with **proteins** or **antibodies**)

RN 7342-41-8 HCAPLUS
 CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



IT **7342-41-8**, [2,2':5',2''-Terthiophene]-5-carboxaldehyde
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of terthiophene **conjugates** with **proteins** or **antibodies**)

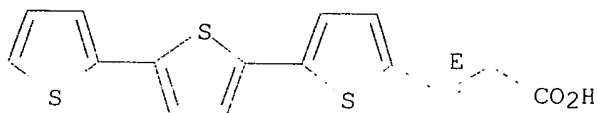
RN 7342-41-8 HCAPLUS
 CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 137584-58-8P 174563-35-0P 174563-36-1P
 174563-40-7P 182629-28-3P 182629-31-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of terthiophene conjugates with proteins or antibodies)

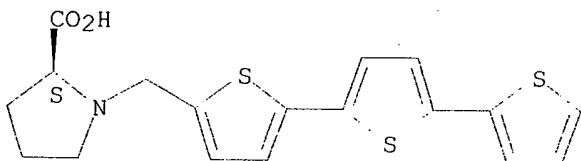
RN 137584-58-8 HCAPLUS
 CN 2-Propenoic acid, 3-[2,2':5',2''-terthiophen]-5-yl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

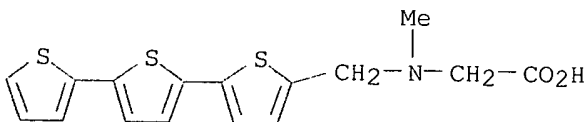


RN 174563-35-0 HCAPLUS
 CN L-Proline, N-([2,2':5',2''-terthiophen]-5-ylmethyl)- (9CI) (CA INDEX NAME)

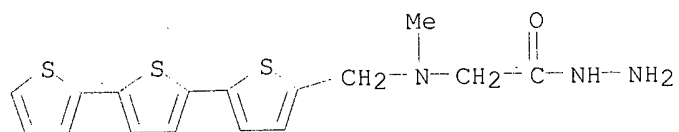
Absolute stereochemistry.



RN 174563-36-1 HCAPLUS
 CN Glycine, N-methyl-N-([2,2':5',2''-terthiophen]-5-ylmethyl)- (9CI) (CA INDEX NAME)

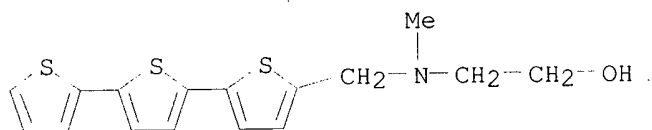


RN 174563-40-7 HCAPLUS
 CN Glycine, N-methyl-N-([2,2':5',2''-terthiophen]-5-ylmethyl)-, hydrazide (9CI) (CA INDEX NAME)



RN 182629-28-3 HCAPLUS

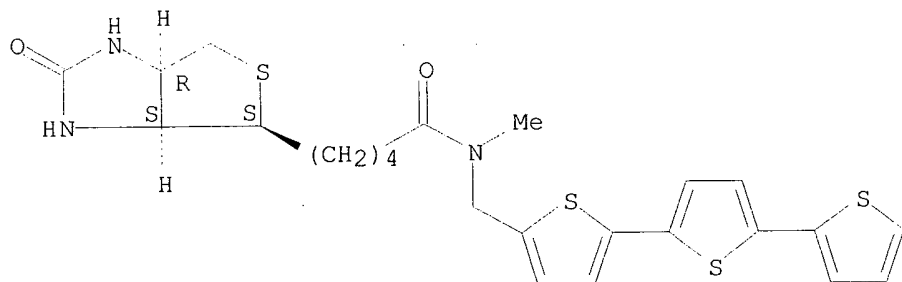
RN	162029-28-3	NCAPLCS			
CN	Ethanol, 2-[methyl([2,2':5',2''-terthiophen]-5-ylmethyl)amino]-	(9CI)	(CA		
INDEX NAME)					



RN 182629-31-8 HCAPLUS

1H-Thieno[3,4-d]imidazole-4-pentanamide, hexahydro-N-methyl-2-oxo-N-
([2,2':5',2''-terthiophen]-5-ylmethyl)-, [3aS-
(3a.alpha.,4.beta.,6a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d ibib abs hitstr 5

L51 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:418719 HCAPLUS

DOCUMENT NUMBER: 125:109072

TITLE: Targeted photolysis of melanoma cells by using an alpha-terthienyl derivative labeled anti-melanoma monoclonal **antibody**

AUTHOR(S): Roncucci, G.; Stefano, A. Di; Soldani, P.; Neri, P.; Neri, D.

CORPORATE SOURCE: Molteni Farmaceutici, Scandicci, 50018, Italy
SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1996), 2625(Photochemistry: Photodynamic Therapy and Other Modalities), 550-560
CODEN: PSISDG; ISSN: 0277-786X

PUBLISHER: SPIE-The International Society for Optical Engineering

DOCUMENT TYPE: Journal

LANGUAGE: English

AB **Antibody** targeted chemotherapy is a relatively new technique which involves the specifically carrier mediated delivery of chemotherapeutic agents to tumors or other pathogens for the treatment of such diseases. **Conjugation of antibodies** with photosensitizers (PSs) can also lead to potential therapeutic agents which combine photodynamic cytotoxicity with specific **antibody** binding. The **antibody** mediated delivery of a photosensitizer mol. and the target destruction upon irradiation by light followed by production of singlet oxygen or other radicals, results in a higher therapeutic ratio compared to the conventional photodynamic therapy (PDT). In this study the naturally occurring PS .alpha.-terthienyl (ATT) was chem. derivatized with an amino group specific reactive side arm and to exploit its toxicity as an effector function suitable for targeted photolysis, covalently **conjugated** to the 225.28S monoclonal **antibody** (mAb) specific for the high mol. wt. melanoma associated antigen (HMW-MAA). The 225-28S-ATT **conjugate** prep. was then tested against the melanoma cell line Colo38 in comparison with HT29 tumor cells, not recognized by 225-28S mAb, as neg. control. The selective uptake of labeled mAb 225-28S-ATT was observed and melanoma cell death following irradiation occurred. In conclusion the 225-28S-ATT **conjugate**, as far as one can judge from the effect on cells grown in vitro, seems a good candidate as a model to test the **antibody** targeted photolysis of melanoma cells for developing specific antimelanoma therapeutic agents.

IT 179339-14-1D, monoclonal **antibody conjugates**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

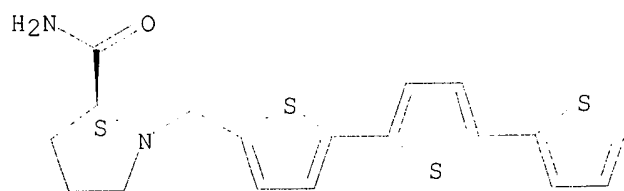
(targeted photolysis of melanoma cells by .alpha.-terthienyl deriv. labeled anti-melanoma monoclonal **antibody**)

RN 179339-14-1 HCAPLUS

CN 2-Pyrrolidinecarboxamide, 1-([2,2':5',2''-terthiophen]-5-ylmethyl)-, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

TRAN 09/871,353



=> d ibib abs hitstr 6

L51 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:398994 HCAPLUS

DOCUMENT NUMBER: 125:80576

TITLE: Study of photoinduced energy and electron transfer in .alpha.-terthienyl-bovine serum albumin **conjugates**: a laser flash photolysis study

AUTHOR(S): Boch, R.; Mohtat, N.; Lear, Y.; Arnason, J. T.; Durst, T.; Scaiano, J. C.

CORPORATE SOURCE: Dep. Chem. Biol., Univ. Ottawa, Ottawa, Can.

SOURCE: Photochemistry and Photobiology (1996), 64(1), 92-99
CODEN: PHCBAP; ISSN: 0031-8655

PUBLISHER: American Society for Photobiology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The photochem. of .alpha.-terthienyl (.alpha.-T) has been examd. in bovine serum albumin (BSA). Freely assocd. and covalently **conjugated** .alpha.-T chromophores show similar behavior toward nonpolar quenchers such as oxygen and benzoquinone but show significant differences in the case of quenching by Me viologen, a water-sol. cationic electron acceptor; in this case, triplet quenching reveals two distinct .alpha.-T populations, attributed to chromophores in sites showing very different accessibility from the aq. phase. Rate consts. for triplet quenching in BSA are generally slower than thos obsd. in homogeneous soln. for free .alpha.-T. For examples, in the case of oxygen, the rate const. is about one order of magnitude smaller when .alpha.-T is assocd. or **conjugated** with the **protein** compared with .alpha.-T in soln. While triplet yields for .alpha.-T are essentially the same in soln. and in the **protein** environment, the yield of detectable singlet oxygen is substantially reduced in the **protein**. This is attributed to a geminate reaction within the **protein** involving singlet oxygen trapping in the vicinity of the generation site.

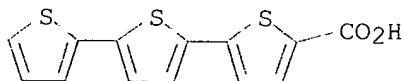
IT 87145-85-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; photoinduced energy and electron transfer in .alpha.-terthienyl-bovine serum albumin **conjugates**: laser flash photolysis study)

RN 87145-85-5 HCAPLUS

CN [2,2':5',2''-Terthiophene]-5-carboxylic acid (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 7

L51 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:171806 HCAPLUS

DOCUMENT NUMBER: 124:232237

TITLE: Preparation of photodynamic .alpha.-terthiophene
conjugates with biocidal properties

INVENTOR(S): Neri, Giovanni; Roncucci, Gabrio

PATENT ASSIGNEE(S): L. Molteni e C. dei Fratelli Alitti Societa' di
Esercizio Societa' per Azioni, Italy

SOURCE: PCT Int. Appl., 37 pp.

CODEN: PIXXD2

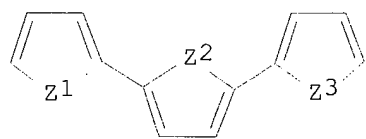
DOCUMENT TYPE: Patent

LANGUAGE: English

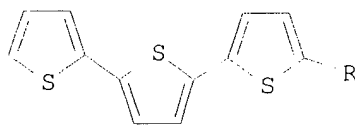
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

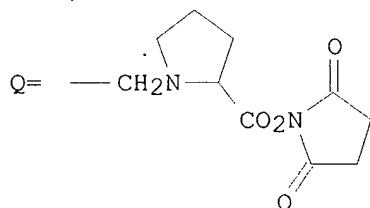
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9532001	A1	19951130	WO 1995-EP1938	19950522
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TT, UA, US, UZ, VN				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2191195	AA	19951130	CA 1995-2191195	19950522
AU 9525662	A1	19951218	AU 1995-25662	19950522
EP 760679	A1	19970312	EP 1995-920073	19950522
EP 760679	B1	20000419		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, PT, SE				
AT 191852	E	20000515	AT 1995-920073	19950522
ES 2147288	T3	20000901	ES 1995-920073	19950522
US 5869051	A	19990209	US 1996-750021	19961122
PRIORITY APPLN. INFO.:			IT 1994-FI95	A 19940523
			WO 1995-EP1938	W 19950522
OTHER SOURCE(S):			MARPAT 124:232237	
GI				



I



II



AB Photodyn. **conjugates** consisting of a carrier mol. and of an org. mol., preferably terthiophene or analogs (I; Z1 - Z3 = S, O), able to

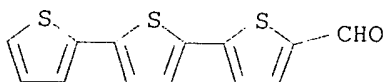
efficiently produce singlet oxygen after irradiation. are prepared. I is suitably derivatized in order to react with an amino, thiol saccharide, histidine, and tyrosine group of the carrier mol. Said carrier mols. are selected from **antibodies**, peptides, heptamers, sugars, or other analogous carriers able to direct the photosensitizer mol. toward a biol. target, e.g. Con A, avidin, biotin, monoclonal **antibody**-anti-Candida albicans, monoclonal **antibody** anti-Herpes simplex virus 1 or 2, and monoclonal **antibody** anti-Rubella virus. Said **conjugates** (e.g. .alpha.-terthiophene **conjugates** with Con A, avidin, biotin, monoclonal **antibody**-anti-Candida albicans, monoclonal **antibody** anti-Herpes simplex virus 1 or 2, and monoclonal **antibody** anti-Rubella virus) are useful either for therapeutic or diagnostic purposes, e.g., as antibacterial, antiviral, antifungal, and antitumor agents. Thus, formylation of 2,2':5',2''-terthiophene (II; R = H) by N-methylformanilide and POCl₃ in CH₂Cl₂ under reflux for 40 h to 5-formyl-.alpha.-terthiophene II (R = CHO) followed reductive alkylation with proline in the presence of NaBH₄ and mol. sieves in MeOH at room temp. for 12 h gave the N-(terthiophenylmethyl)L-proline II (R = CH₂-Pro-OH), which was esterified with N-hydroxysuccinimide using DCC in DMF/CH₂Cl₂ at room temp. for 20 h to give the active ester II (R = Q). The latter compd. was coupled with Con A (ConA) in 100 mM phosphate buffer (pH 8) to give the ConA-.alpha.-terthiophene **conjugate**. Suspension of Candida albicans and Saccharomyces cerevisiae was incubated in the dark with the latter **conjugate** at 3 .times. 10⁻⁸ M for 0.5 h and then irradiated at 350 nm for 30 min and incubated in the dark for 24 h at 33.degree.. The growth of the treated fungi was completely inhibited. Monoclonal **antibodies** against Herpes simplex virus 1 or 2, Candida albicans, anti-Rubella virus, and 225-28S.

IT 7342-41-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (antibacterial agent by itself; prepn. of photodynamic .alpha.-terthiophene **conjugates** for producing singlet oxygen as biocides or diagnostics)

RN 7342-41-8 HCAPLUS

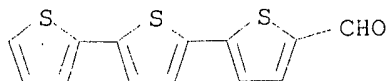
CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)

IT 7342-41-8DP, **conjugates** with bovine serum albumin

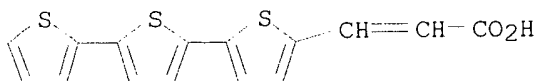
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of photodynamic .alpha.-terthiophene **conjugates** for producing singlet oxygen as biocides or diagnostics)

RN 7342-41-8 HCAPLUS

CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)

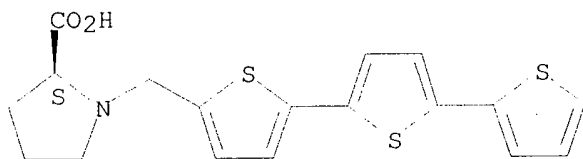


IT 138024-51-8P 174563-35-0P 174563-36-1P
 174563-40-7P 174563-42-9P 174563-43-0P
 174563-47-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. of photodynamic .alpha.-terthiophene **conjugates** for
 producing singlet oxygen as biocides or diagnostics)
 RN 138024-51-8 HCAPLUS
 CN 2-Propenoic acid, 3-[2,2':5',2''-terthiophen]-5-yl- (9CI) (CA INDEX NAME)

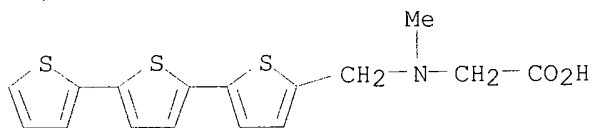


RN 174563-35-0 HCAPLUS
 CN L-Proline, N-([2,2':5',2''-terthiophen]-5-ylmethyl)- (9CI) (CA INDEX NAME)

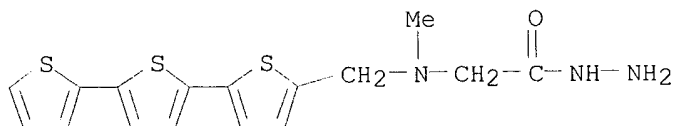
Absolute stereochemistry.



RN 174563-36-1 HCAPLUS
 CN Glycine, N-methyl-N-([2,2':5',2''-terthiophen]-5-ylmethyl)- (9CI) (CA INDEX NAME)



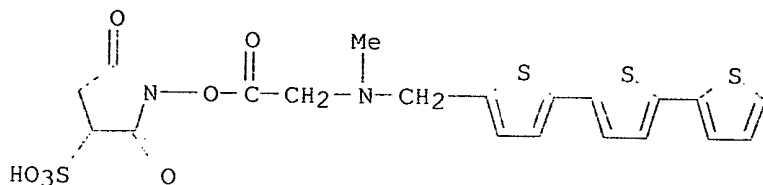
RN 174563-40-7 HCAPLUS
 CN Glycine, N-methyl-N-([2,2':5',2''-terthiophen]-5-ylmethyl)-, hydrazide
 (9CI) (CA INDEX NAME)



TRAN 09/871,353

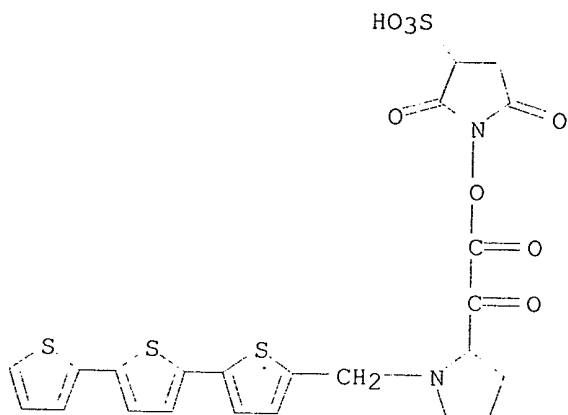
RN 174563-42-9 HCAPLUS

CN 3-Pyrrolidinesulfonic acid, 1-[[[methyl([2,2':5',2''-terthiophen]-5-ylmethyl)amino]acetyl]oxy]-2,5-dioxo- (9CI) (CA INDEX NAME)



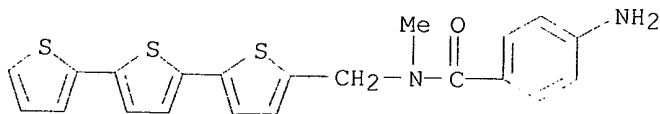
RN 174563-43-0 HCAPLUS

CN 3-Pyrrolidinesulfonic acid, 2,5-dioxo-1-[[oxo[1-([2,2':5',2''-terthiophen]-5-ylmethyl)-2-pyrrolidinyl]acetyl]oxy]- (9CI) (CA INDEX NAME)



RN 174563-47-4 HCAPLUS

CN Benzamide, 4-amino-N-methyl-N-([2,2':5',2''-terthiophen]-5-ylmethyl)- (9CI) (CA INDEX NAME)



TRAN 09/871,353

for explanation of this
d que see L51
g very display

=> d que 155

```

L1      19 SEA FILE=HCAPLUS ABB=ON PLU=ON CIPRIANI F?/AU
L2      135 SEA FILE=HCAPLUS ABB=ON PLU=ON GIGLI G?/AU
L3      377 SEA FILE=HCAPLUS ABB=ON PLU=ON CINGOLANI R?/AU
L4      48 SEA FILE=HCAPLUS ABB=ON PLU=ON FAVARETTO L?/AU
L5      59 SEA FILE=HCAPLUS ABB=ON PLU=ON ZAMBIANCHI M?/AU
L6      78 SEA FILE=HCAPLUS ABB=ON PLU=ON SOTGIU G?/AU
L7      71 SEA FILE=HCAPLUS ABB=ON PLU=ON CITRO G?/AU
L8      132 SEA FILE=HCAPLUS ABB=ON PLU=ON BARBARELLA G?/AU
L9      734 SEA FILE=HCAPLUS ABB=ON PLU=ON (L1 OR L2 OR L3 OR L4 OR L5
      OR L6 OR L7 OR L8)
L10     54 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 AND THIOPHENE
L11     30 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 AND OLIGOMER?
L12     5 SEA FILE=HCAPLUS ABB=ON PLU=ON L11 AND (THIOPHENE OLIGOMER)/T
      I
L13     24 SEA FILE=REGISTRY ABB=ON PLU=ON (376393-41-8/BI OR 376393-42-
      9/BI OR 376393-43-0/BI OR 376393-44-1/BI OR 492-97-7/BI OR
      111372-97-5/BI OR 111744-23-1/BI OR 113386-74-6/BI OR 116159-99
      -0/BI OR 118347-89-0/BI OR 127236-47-9/BI OR 127236-48-0/BI OR
      127473-73-8/BI OR 127473-74-9/BI OR 127473-75-0/BI OR 139747-07
      -2/BI OR 139747-08-3/BI OR 14762-74-4/BI OR 201604-95-7/BI OR
      201604-98-0/BI OR 25233-34-5/BI OR 376393-45-2/BI OR 5632-29-1/
      BI OR 67984-20-7/BI)
L14     4 SEA FILE=HCAPLUS ABB=ON PLU=ON L12 AND L13
L15     5 SEA FILE=HCAPLUS ABB=ON PLU=ON L12 OR L14
L16     STR

```

11

Q
||
||

Hy[^]Hy[^]Hy[^] G1 4 Q[~]C[~] A⁼⁼C⁼⁼ Q⁼⁼C⁼⁼N
1 2 3 @5 @6 7 @8 9 10 @12

VAR G1=5/6/8/12/NH2/OH/SH/SO3H/SO2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

GGCAT IS MCY UNS AT 2

GGCAT IS MCY UNS AT 3

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E4 C E1 S AT 1

ECOUNT IS E4 C E1 S AT 2

ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L17 289013 SEA FILE=REGISTRY ABB=ON PLU=ON 16.145.3/RID

L19 STR

Hy[^]Hy[^]Hy[^]
1 2 3

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

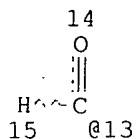
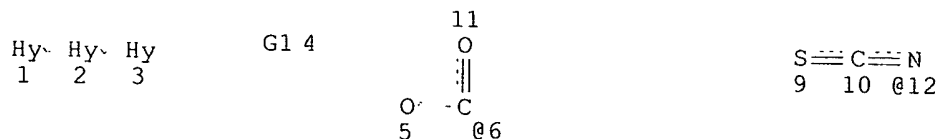
GGCAT IS MCY UNS AT 2

GGCAT IS MCY UNS AT 3
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS E4 C E1 S AT 1
 ECOUNT IS E4 C E1 S AT 2
 ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

L21 5115 SEA FILE=REGISTRY SUB=L17 SSS FUL L19
 L23 2293 SEA FILE=REGISTRY SUB=L21 SSS FUL L16
 L26 STR



VAR G1=OH/SH/NH2/13/6/12

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 5
 DEFAULT MLEVEL IS ATOM
 GGCAT IS MCY UNS AT 1
 GGCAT IS MCY UNS AT 2
 GGCAT IS MCY UNS AT 3
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS E4 C E1 S AT 1
 ECOUNT IS E4 C E1 S AT 2
 ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L27 1357 SEA FILE=REGISTRY SUB=L23 SSS FUL L26
 L28 476 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 3 16.145.3/RID
 L29 166 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 4 16.145.3/RID
 L30 104 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 5 16.145.3/RID
 L31 746 SEA FILE=REGISTRY ABB=ON PLU=ON (L28 OR L29 OR L30)
 L32 674 SEA FILE=REGISTRY ABB=ON PLU=ON L31 AND NC=1 NOT ("DIAZO" OR
 F/ELS)
 L33 23948 SEA FILE=REGISTRY ABB=ON PLU=ON 2 16.145.3/RID
 L35 2996 SEA FILE=REGISTRY ABB=ON PLU=ON L33 AND "BITHIOPHENE"
 L38 662 SEA FILE=REGISTRY ABB=ON PLU=ON L35 AND ("HYDROXY" OR
 "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORMYL" OR "ISOTHIOCYANATO"
 OR "THIOL" OR "AMINO" OR "CARBOXYLIC") NOT "ESTER"
 L39 584 SEA FILE=REGISTRY ABB=ON PLU=ON L38 AND NC=1
 L40 451 SEA FILE=REGISTRY ABB=ON PLU=ON L39 NOT "AZO"
 L41 287 SEA FILE=HCAPLUS ABB=ON PLU=ON L32

TRAN 09/871,353

L42 455 SEA FILE=HCAPLUS ABB=ON PLU=ON L40
L43 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L41(L)?CONJUGAT?
L44 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L42(L)?CONJUGAT?
L45 26 SEA FILE=HCAPLUS ABB=ON PLU=ON L43 OR L44
L46 25 SEA FILE=HCAPLUS ABB=ON PLU=ON L45 NOT L15
L47 3042811 SEA FILE=HCAPLUS ABB=ON PLU=ON ANTIBOD? OR FLUORESC?(3A)MARKE
R OR PROTEIN OR DNA OR NUCLEIC OR OLIGONUC? OR HORMON? OR DRUG
OR MEDICINE OR NEUROTRANSMITTER
L48 121828 SEA FILE=HCAPLUS ABB=ON PLU=ON SPECTROFLUORIMETRY OR
CYTOMETRY OR FLUORESCENCE(W)MICROSCO? OR GEL ELECTROPHOR?
L49 40 SEA FILE=HCAPLUS ABB=ON PLU=ON (L41 OR L42) AND (L47 OR L48)

L50 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L49 AND ?CONJUGAT?
L51 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L50 NOT L15
L52 20 SEA FILE=HCAPLUS ABB=ON PLU=ON L46 NOT L51
L53 18 SEA FILE=HCAPLUS ABB=ON PLU=ON L52 NOT PATENT/DT
L54 17 SEA FILE=HCAPLUS ABB=ON PLU=ON L53 AND PD<20010530
L55 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L54 AND (VISIBLE(3A)(UV OR
ULTRAVIOET))

4 cites

=> d ibib abs hitstr 1

L55 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:527050 HCAPLUS

DOCUMENT NUMBER: 135:288881

TITLE: Synthesis, structures and nonlinear optical properties of novel D-.pi.-A chromophores: intramolecular charge transfer from 1,3-dithiole or ferrocene moieties to polynitrofluorene or dicyanomethylene moieties through conjugated linkers

AUTHOR(S): Moore, Adrian J.; Chesney, Antony; Bryce, Martin R.; Batsanov, Andrei S.; Kelly, Janet F.; Howard, Judith A. K.; Perepichka, Igor F.; Perepichka, Dmitrii F.; Meshulam, Guilia; Berkovic, Garry; Kotler, Zvi; Mazor, Royi; Khodorkovsky, Vladimir

CORPORATE SOURCE: Department of Chemistry, University of Durham, Durham, DH1 3LE, UK

SOURCE: European Journal of Organic Chemistry (2001), (14), 2671-2687

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:288881

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Electron donor-.pi.-acceptor chromophores, e.g., I (R = MeS) and II (R = NO₂ (38a), CO₂Me (38b), CO₂(CH₂CH₂O)3Me (38c), Fc = ferrocenyl), were synthesized. The donor units are 1,3-dithiole and ferrocene; conjugated ethylenic, Ph, phenylenevinylene, thienyl, bithienyl, terthienyl, or thienylenevinylene linkers act as a central .pi.-electron relay unit, and dicyanomethylene and polynitrofluorene groups as the acceptor unit. The electronic absorption spectra display a broad low-energy intramol. charge transfer band in the visible region (500-700 nm) the energy (hvICT .apprxeq. 1.7-2.5 eV) and intensity (.epsilon. .apprxeq. 5000-50000 m⁻¹cm⁻¹) of which depend substantially on the nature of both D and A moieties and on the structure of the linker unit. Nonlinear optical properties were evaluated using the EFISH technique: the highest .mu..beta.(0) values are obsd. for 38b [(900 .+- . 300).times.10⁻⁴⁸ esu] and 42 (shown as III) [(1800 .+- . 300).times.10⁻⁴⁸ esu] establishing that polynitrofluorene is a promising acceptor terminal moiety in this context. The mol. and electronic structures of 49 and 50 (shown as IV and I (R = H), resp.) were calcd. by the RHF/6-31G(d)//RHF/6-31G(d) ab initio method. The HOMO is located mostly in the 1,3-dithiolium ring, and the LUMO mostly at the dicyanomethylene fragment (and the Ph ring of 50) although the electronic population at C2 of the 1,3-dithiolium rings is also considerable. The x-ray crystal structures of 9, 18 (shown as V and VI, resp.), and (E)-p-[(NC)2C:CH]C6H4CH:CHFc (27), were reported. In all three structures the conjugated .pi.-systems are effectively planar with extensive .pi.-electron delocalization between the donor and acceptor moieties. The planar conformation of 18 gives rise to a close intramol. S-S contact of 3.095(3) .ANG. between the dithiole and thiophene units.

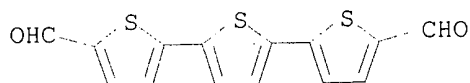
IT 13130-50-2 32364-72-0, 2,2'-Bithiophene-5,5'-dialdehyde
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. and nonlinear optical properties of D-.pi.-A chromophores from

TRAN 09/871,353

1,3-dithiole or ferrocene moieties contg. polynitrofluorene or dicyanomethylene moieties through **conjugated** linkers)

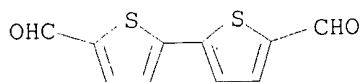
RN 13130-50-2 HCAPLUS

CN [2,2':5',2''-Terthiophene]-5,5''-dicarboxaldehyde (8CI, 9CI) (CA INDEX NAME)



RN 32364-72-0 HCAPLUS

CN [2,2'-Bithiophene]-5,5'-dicarboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



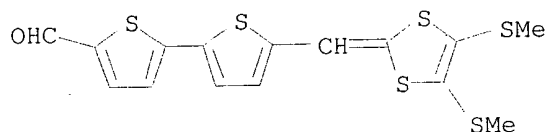
IT 365210-82-8P 365210-83-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and nonlinear optical properties of D-.pi.-A chromophores from 1,3-dithiole or ferrocene moieties contg. polynitrofluorene or dicyanomethylene moieties through **conjugated** linkers)

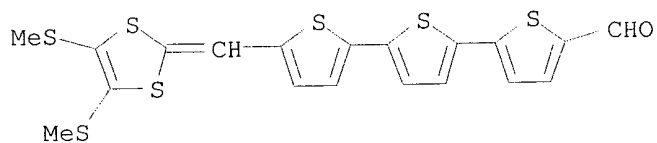
RN 365210-82-8 HCAPLUS

CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde, 5'-[[4,5-bis(methylthio)-1,3-dithiol-2-ylidene]methyl]- (9CI) (CA INDEX NAME)



RN 365210-83-9 HCAPLUS

CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde, 5'-[[4,5-bis(methylthio)-1,3-dithiol-2-ylidene]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

109

THERE ARE 109 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L55 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2002 ACS

CC 29-12 (Organometallic and Organometalloidal Compounds)

- Section cross-reference(s): 25, 27, 28, 73, 75
- ST crystal structure ferrocene thiophene phenylene thiophenylene dicyanomethylene deriv; nonlinear optical property dithiole ferrocene polynitrofluorene dicyanomethylene deriv prepn; electronic structure dithiolylidene dicyanomethylene deriv; HOMO LUMO dithiolylidene dicyanomethylene deriv; mol structure ferrocene thiophene phenylene thiophenylene dicyanomethylene deriv; charge transfer intramol dithiole ferrocene polynitrofluorene dicyanomethylene deriv; RHF MO calcn dithiolylidene dicyanomethylene deriv; safety exothermic reaction ferrocenylpentadienal prepn
- IT Electron delocalization
(between donor and acceptor moieties in dithiolylidene and dicyanomethylene-contg. model electron donor-.pi.-acceptor moieties)
- IT Safety
(hazard due to exothermic reaction during prepn. ferrocenylpentadienal as intermediate in prepn. of D-.pi.-A chromophore contg. ferrocene and dicyano moieties)
- IT Electron transfer
(intramol.; synthesis, structures and nonlinear optical properties of novel D-.pi.-A chromophores and intramol. charge transfer from 1,3-dithiole or ferrocene moieties to polynitrofluorene or dicyanomethylene moieties through conjugated linkers)
- IT HOMO (molecular orbital)
LUMO (molecular orbital)
RHF (molecular orbital)
(of dithiolylidene and dicyanomethylene-contg. model electron donor-.pi.-acceptor model chromophores)
- IT Electronic structure
Second-order nonlinear optical properties
UV and visible spectra
(of electron donor-.pi.-acceptor chromophores contg. dithiole, ferrocene, polynitrofluorene, and dicyanomethylene moieties)
- IT Crystal structure
Molecular structure
(of ferrocene- and dithiole-contg. chromophores contg. phenylene or thiophenylene and dicyanomethylene moieties)
- IT Molecular orbital
(optimized; of dithiolylidene and dicyanomethylene-contg. model electron donor-.pi.-acceptor model chromophores)
- IT Chromophores
(synthesis, structures and nonlinear optical properties of novel D-.pi.-A chromophores and intramol. charge transfer from 1,3-dithiole or ferrocene moieties to polynitrofluorene or dicyanomethylene moieties through conjugated linkers)
- IT 365210-95-3 365210-96-4
RL: PRP (Properties)
(electronic and mol. structures calcd. by RHF ab initio method)
- IT 223134-50-7P 241161-37-5P 241161-39-7P 241161-47-7P 365210-81-7P
365210-84-0P 365210-85-1P 365210-86-2P 365210-87-3P 365210-88-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and electronic absorption spectra of)
- IT 241161-53-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and electronic absorption spectra of)
- IT 365210-94-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and nonlinear optical properties of)
- IT 329246-94-8P 329247-02-1P
RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic

- preparation); PREP (Preparation)
 (prepn. and nonlinear optical properties of D-.pi.-A chromophores from
 1,3-dithiole or ferrocene moieties contg. polynitrofluorene or
 dicyanomethylene moieties through conjugated linkers)
- IT 109-77-3P, Malononitrile 300710-65-0P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and nonlinear optical properties of D-.pi.-A chromophores from
 1,3-dithiole or ferrocene moieties contg. polynitrofluorene or
 dicyanomethylene moieties through conjugated linkers)
- IT 98243-44-8P
 RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic
 preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and nonlinear optical properties of D-.pi.-A chromophores from
 1,3-dithiole or ferrocene moieties contg. polynitrofluorene or
 dicyanomethylene moieties through conjugated linkers)
- IT 623-27-8, 1,4-Benzenedicarboxaldehyde 932-95-6, 2,5-
 Thiophenedicarbaldehyde 1271-47-2, Ferrocenylethyne 12093-10-6,
 Ferrocenecarboxaldehyde 13130-50-2 20430-33-5,
 (4-Cyanobenzyl)triphenylphosphonium chloride 22411-59-2,
 p-(Diethylamino)cinnamaldehyde 32364-72-0, 2,2'-Bithiophene-5,5'-
 dialdehyde 32914-67-3, (Ferrocenylmethyl)triphenylphosphonium iodide
 56637-71-9 185426-82-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. and nonlinear optical properties of D-.pi.-A chromophores from
 1,3-dithiole or ferrocene moieties contg. polynitrofluorene or
 dicyanomethylene moieties through **conjugated** linkers)
- IT 98243-45-9P 123931-08-8P 183384-17-0P 223134-46-1P 365210-76-0P
 365210-78-2P 365210-79-3P **365210-82-8P 365210-83-9P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and nonlinear optical properties of D-.pi.-A chromophores from
 1,3-dithiole or ferrocene moieties contg. polynitrofluorene or
 dicyanomethylene moieties through **conjugated** linkers)
- IT 29210-71-7, 2,4,5,7-Tetranitrofluorene 164297-32-9, 2,5,7-Trinitro-4-
 methoxycarbonylfluorene 226419-15-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. and nonlinear optical properties of D-.pi.-A electron
 chromophores from 1,3-dithiole or ferrocene moieties contg.
 polynitrofluorene or dicyanomethylene moieties through conjugated
 linkers)
- IT 123931-07-7P
 RL: BYP (Byproduct); REM (Removal or disposal); PREP (Preparation); PROC
 (Process)
 (prepn. of)
- IT 365210-90-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
- IT 241161-50-2P 241161-57-9P 241161-58-0P 365210-77-1P 365210-89-5P
 365210-92-0P 365210-93-1P 365210-97-5P 365210-98-6P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn., electronic absorption spectra, and nonlinear optical
 properties of)
- IT 196696-74-9P 223134-55-2P 365210-80-6P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn., electronic absorption spectra, nonlinear optical properties,
 and crystal structure of)
- IT 1271-67-6P, Ferrocenyl(formyl)acetylene
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (prepn., reaction with fluorene deriv., and electronic absorption

- spectra of)
- IT 1272-17-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and caution due to exothermic reaction during prepn. as
intermediate in prepn. of D-.pi.-A chromophore contg. ferrocene and
dicyano moieties)
- IT 365210-91-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and electronic absorption spectra of)

=> d ibib abs hitstr 2

L55 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:498564 HCAPLUS

DOCUMENT NUMBER: 133:252378

TITLE: Mixed .pi.-conjugated oligomers of thiophene and 3,4-ethylenedioxythiophene (EDOT)

AUTHOR(S): Turbiez, M.; Frere, P.; Blanchard, P.; Roncali, J.

CORPORATE SOURCE: Ingenierie Moleculaire et Materiaux Organiques, UMR-CNRS 6501, Angers, 49045, Fr.

SOURCE: Tetrahedron Letters (2000), 41(29), 5521-5525

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:252378

AB Conjugated oligomers based on various combinations of thiophene and 3,4-ethylenedioxythiophene (EDOT) moieties were synthesized. Comparison of the optical and electrochem. properties shows that the introduction of a bis-EDOT core in the middle of the system produces a decrease of the HOMO-LUMO gap which is attributed to an enhancement of the planarity and rigidity of the .pi.-conjugated system.

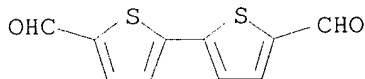
IT 32364-72-0, 2,2'-Bithiophene-5,5'-dicarboxaldehyde

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of mixed **conjugated** oligomers of thiophene and ethylenedioxythiophene)

RN 32364-72-0 HCAPLUS

CN [2,2'-Bithiophene]-5,5'-dicarboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ind 2

L55 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2002 ACS

CC 28-11 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 22

ST conjugated thiophene oligomer prepn electronic property; oxidn potential
UV conjugated thiophene oligomer

IT Oxidation potential

UV and visible spectra

(of mixed conjugated oligomers of thiophene and ethylenedioxythiophene)

IT 250726-94-4P 250726-96-6P 295358-38-2P 295358-39-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(oxidn. potential and UV spectra)

IT 1003-09-4, 2-Bromothiophene 4805-22-5, 5,5'-Dibromo-2,2'-bithiophene

32364-72-0, 2,2'-Bithiophene-5,5'-dicarboxaldehyde 126213-50-1

175922-79-9 195602-17-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of mixed **conjugated** oligomers of thiophene and ethylenedioxythiophene)

TRAN 09/871,353

IT 98-03-3P, 2-Thienaldehyde 199168-63-3P 295358-40-6P 295358-41-7P
295358-42-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. of mixed conjugated oligomers of thiophene and
ethylenedioxythiophene)

=> d ibib abs hitstr 3

L55 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:457921 HCAPLUS

DOCUMENT NUMBER: 133:193729

TITLE: Redox States of Well-Defined .pi.-Conjugated
Oligothiophenes Functionalized with Poly(benzyl ether)
DendronsAUTHOR(S): Apperloo, Joke J.; Janssen, Rene A. J.; Malenfant,
Patrick R. L.; Groenendaal, Lambertus; Frechet, Jean
M. J.CORPORATE SOURCE: Laboratory for Macromolecular and Organic Chemistry,
Eindhoven University of Technology, Eindhoven, 5600
MB, Neth.SOURCE: Journal of the American Chemical Society (2000
, 122(29), 7042-7051

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The redox states of a series of well-defined hybrid dendrimers based on oligothiophene cores and poly(benzyl ether) dendrons have been studied using cyclic voltammetry and variable-temp. **UV/visible** /near-IR spectroscopy. The oxidn. potentials and the electronic transitions of the neutral, singly oxidized, and doubly oxidized states of these novel hybrid materials have been detd. as a function of oligothiophene conjugation length varying between 4 and 17 repeat units. The attachment of poly(benzyl ether) dendritic wedges at the termini of these lengthy oligothiophenes considerably enhances their soly., thus enabling the first detailed investigation of the electronic structure of oligothiophenes having 11 and 17 repeat units with minimal .beta.-substitution. In the case of the undecamer and heptadecamer, we find that the dicationic state consists of two individual polarons, rather than a single bipolaron. The effect of the dendritic poly(benzyl ether) solubilizers on the properties of the redox states varies with the oligothiophene length and dendron size. More specifically, we observe a kinetic limit to the electrochem. oxidn. of the oligothiophene core when the dendron is large compared to the electrophore. Finally, we have obsd. the first example of self-complexation of cation radicals via .pi.-dimerization leading to the formation of dendritic supramol. assemblies.

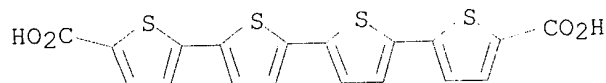
IT 288861-01-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)(redox states of .pi.-conjugated oligothiophenes
functionalized with poly(benzyl ether) dendrons)

RN 288861-01-8 HCAPLUS

CN [2,2':5',2'':5'',2''':5'''-Quaterthiophene]-5,5'''-dicarboxylic acid (9CI) (CA

INDEX NAME)



REFERENCE COUNT:

63

THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

TRAN 09/871,353

=> d ibib abs hitstr 4

L55 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:195129 HCAPLUS

DOCUMENT NUMBER: 124:233307

TITLE: Synthesis and Characterization of A New Conjugated

Aromatic Poly(azomethine) Derivative Based on the

3',4'-Dibutyl-.alpha.-Terthiophene Building Block

AUTHOR(S):

Wang, Chenggang; Shieh, Seaver; LeGoff, Eugene;
Kanatizidis, Mercouri G.

CORPORATE SOURCE:

Department of Chemistry, Michigan State University,
East Lansing, MI, 48824, USA

SOURCE:

Macromolecules (1996), 29(9), 3147-56

CODEN: MAMOBX; ISSN: 0024-9297

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB A new conjugated arom. poly(azomethine) deriv., poly(3',4'-dibutyl-.alpha.-terthiophene-azomethine-1,4-phenylene-azomethine) (PBTPI), has been prepd. by polycondensation of 2,5''-diformyl-3',4'-dibutyl-2,2':5',2''-terthiophene with 1,4-phenylenediamine under the ethanothormal conditions. The red polycryst. PBTPI was characterized by X-ray diffraction, NMR, FTIR, **UV-visible**-near-IR, photoluminescence, and ESR spectroscopies. PBTPI is partially sol. in THF, giving an orange soln. with an absorption max. (.lambda.max) of 457 nm. In the solid state, PBTPI has an optical band gap of 2.06 eV, which is one of the lowest among poly(azomethines), and is highly sensitive to a strong acid environment. Protonation yields a blue polymer with an optical band gap of 1.61 eV. The polymer is completely sol. in concd. sulfuric acid and nitromethane contg. Lewis acids (e.g., AlCl₃), giving blue solns. with .lambda.max of 656 and 638 nm, resp. Iodine-doped PBTPI shows low elec. cond. at the order of 10⁻⁷-10⁻⁸ S/cm. The properties of PBTPI are compared to other, previously characterized, related polymers.

IT

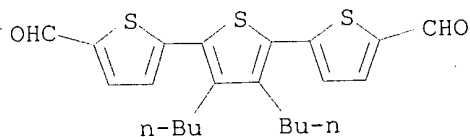
169565-01-9P, 2,5''-Diformyl-3',4'-dibutyl-2,2':5',2''-terthiophene

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(monomer; prepn. and optical and elec. properties of **conjugated** arom. poly(azomethine) deriv. based on the 3',4'-dibutyl-.alpha.-terthiophene building block)

RN 169565-01-9 HCAPLUS

CN [2,2':5',2''-Terthiophene]-5,5''-dicarboxaldehyde, 3',4'-dibutyl- (9CI)
(CA INDEX NAME)



TRAN 09/871,353

See L51 query display
for explanation of
this d que

=> d que 156

L1 19 SEA FILE=HCAPLUS ABB=ON PLU=ON CIPRIANI F?/AU
L2 135 SEA FILE=HCAPLUS ABB=ON PLU=ON GIGLI G?/AU
L3 377 SEA FILE=HCAPLUS ABB=ON PLU=ON CINGOLANI R?/AU
L4 48 SEA FILE=HCAPLUS ABB=ON PLU=ON FAVARETTO L?/AU
L5 59 SEA FILE=HCAPLUS ABB=ON PLU=ON ZAMBIANCHI M?/AU
L6 78 SEA FILE=HCAPLUS ABB=ON PLU=ON SOTGIU G?/AU
L7 71 SEA FILE=HCAPLUS ABB=ON PLU=ON CITRO G?/AU
L8 132 SEA FILE=HCAPLUS ABB=ON PLU=ON BARBARELLA G?/AU
L9 734 SEA FILE=HCAPLUS ABB=ON PLU=ON (L1 OR L2 OR L3 OR L4 OR L5
OR L6 OR L7 OR L8)
L10 54 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 AND THIOPHENE
L11 30 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 AND OLIGOMER?
L12 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L11 AND (THIOPHENE OLIGOMER)/T
I
L13 24 SEA FILE=REGISTRY ABB=ON PLU=ON (376393-41-8/BI OR 376393-42-
9/BI OR 376393-43-0/BI OR 376393-44-1/BI OR 492-97-7/BI OR
111372-97-5/BI OR 111744-23-1/BI OR 113386-74-6/BI OR 116159-99
-0/BI OR 118347-89-0/BI OR 127236-47-9/BI OR 127236-48-0/BI OR
127473-73-8/BI OR 127473-74-9/BI OR 127473-75-0/BI OR 139747-07
-2/BI OR 139747-08-3/BI OR 14762-74-4/BI OR 201604-95-7/BI OR
201604-98-0/BI OR 25233-34-5/BI OR 376393-45-2/BI OR 5632-29-1/
BI OR 67984-20-7/BI)
L14 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L12 AND L13
L15 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L12 OR L14
L16 STR °

11

Q

||

Hy^Hy^Hy G1 4 Q~C A=C Q=C=N
1 2 3 @5 @6 7 @8 9 10 @12

VAR G1=5/6/8/12/NH2/OH/SH/SO3H/SO2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

GGCAT IS MCY UNS AT 2

GGCAT IS MCY UNS AT 3

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E4 C E1 S AT 1

ECOUNT IS E4 C E1 S AT 2

ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L17 289013 SEA FILE=REGISTRY ABB=ON PLU=ON 16.145.3/RID

L19 STR °

Hy^Hy^Hy
1 2 3

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

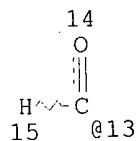
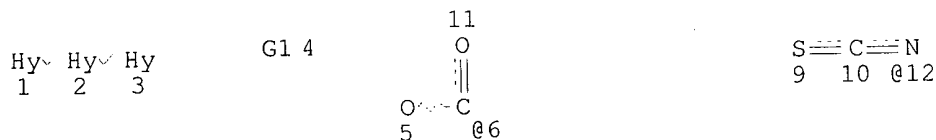
GGCAT IS MCY UNS AT 1

GGCAT IS MCY UNS AT 2

GGCAT IS MCY UNS AT 3
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS E4 C E1 S AT 1
 ECOUNT IS E4 C E1 S AT 2
 ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE
 L21 5115 SEA FILE=REGISTRY SUB=L17 SSS FUL L19
 L23 2293 SEA FILE=REGISTRY SUB=L21 SSS FUL L16
 L26 STR



VAR G1=OH/SH/NH2/13/6/12

NODE ATTRIBUTES:
 CONNECT IS E1 RC AT 5
 DEFAULT MLEVEL IS ATOM
 GGCAT IS MCY UNS AT 1
 GGCAT IS MCY UNS AT 2
 GGCAT IS MCY UNS AT 3
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS E4 C E1 S AT 1
 ECOUNT IS E4 C E1 S AT 2
 ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
 L27 1357 SEA FILE=REGISTRY SUB=L23 SSS FUL L26
 L28 476 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 3 16.145.3/RID
 L29 166 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 4 16.145.3/RID
 L30 104 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 5 16.145.3/RID
 L31 746 SEA FILE=REGISTRY ABB=ON PLU=ON (L28 OR L29 OR L30)
 L32 674 SEA FILE=REGISTRY ABB=ON PLU=ON L31 AND NC=1 NOT ("DIAZO" OR
 F/ELS)
 L33 23948 SEA FILE=REGISTRY ABB=ON PLU=ON 2 16.145.3/RID
 L35 2996 SEA FILE=REGISTRY ABB=ON PLU=ON L33 AND "BITHIOPHENE"
 L38 662 SEA FILE=REGISTRY ABB=ON PLU=ON L35 AND ("HYDROXY" OR
 "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORMYL" OR "ISOTHIOCYANATO"
 OR "THIOL" OR "AMINO" OR "CARBOXYLIC") NOT "ESTER"
 L39 584 SEA FILE=REGISTRY ABB=ON PLU=ON L38 AND NC=1
 L40 451 SEA FILE=REGISTRY ABB=ON PLU=ON L39 NOT "AZO"
 L41 287 SEA FILE=HCAPLUS ABB=ON PLU=ON L32

TRAN 09/871,353

L42 455 SEA FILE=HCAPLUS ABB=ON PLU=ON L40
L43 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L41(L)?CONJUGAT?
L44 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L42(L)?CONJUGAT?
L45 26 SEA FILE=HCAPLUS ABB=ON PLU=ON L43 OR L44
L46 25 SEA FILE=HCAPLUS ABB=ON PLU=ON L45 NOT L15
L47 3042811 SEA FILE=HCAPLUS ABB=ON PLU=ON ANTIBOD? OR FLUORESC?(3A)MARKE
OR PROTEIN OR DNA OR NUCLEIC OR OLIGONUC? OR HORMON? OR DRUG
OR MEDICINE OR NEUROTRANSMITTER
L48 121828 SEA FILE=HCAPLUS ABB=ON PLU=ON SPECTROFLUORIMETRY OR
CYTOMETRY OR FLUORESCENCE(W)MICROSCO? OR GEL ELECTROPHOR?
L49 40 SEA FILE=HCAPLUS ABB=ON PLU=ON (L41 OR L42) AND (L47 OR L48)
L50 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L49 AND ?CONJUGAT?
L51 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L50 NOT L15
L52 20 SEA FILE=HCAPLUS ABB=ON PLU=ON L46 NOT L51
L56 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L52 AND PATENT/DT

2 patents.

=> d ibib abs hitstr 1

L56 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2002:172353 HCAPLUS
 DOCUMENT NUMBER: 136:238802
 TITLE: Second-order nonlinear optical chromophores containing
 dioxine and/or bithiophene as conjugate bridge and
 devices incorporating the same
 INVENTOR(S): Wang, Chuanguang; Zhang, Cheng; Fetterman, Harold R.;
 Steier, William; Michael, Joseph
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 16 pp., Cont.-in-part of U. S.
 Ser. No. 488,422.
 CODEN: USXXCO
 DOCUMENT TYPE: **Patent**
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 7
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002027220	A1	20020307	US 2001-898625	20010703
US 6067186	A	20000523	US 1998-122806	19980727
US 6361717	B1	20020326	US 2000-488422	20000120
US 6348992	B1	20020219	US 2000-551685	20000418
PRIORITY APPLN. INFO.:			US 1998-122806	A2 19980727
			US 2000-488422	A2 20000120
			US 2000-546930	A2 20000411
			US 2000-551685	A2 20000418

OTHER SOURCE(S): MARPAT 136:238802
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Nonlinear optical devices (e.g., electrooptical modulators, phase shifters) comprising an active element formed from a chromophore including an electron donor group, an electron acceptor group, and a bridge structure between the electron donor group and the electron acceptor group are described in which the chromophores is described by the general formula I, the bridge structure is described by the general formula II, or the electron donor group and the bridge structure are described by the general formula III (A = CH₂ or O; B = is an electron acceptor; and R = independently selected H, F, or a perhalogenated, halogenated, or nonhalogenated C1-30 aliph. or arom. group functionalized with .gtoreq.0 hydroxy, ether, ester, amino, silyl, and siloxy groups).

IT 392662-52-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

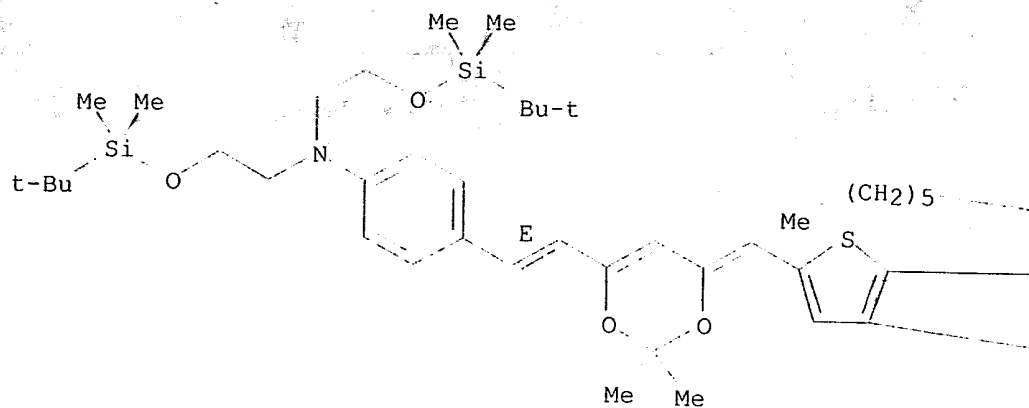
(nonlinear optical devices employing second-order nonlinear optical chromophores contg. dioxine and/or bithiophene as **conjugate** bridge)

RN 392662-52-1 HCAPLUS

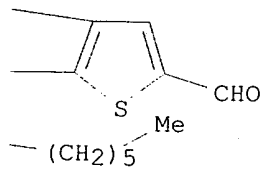
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-[[6-[(1E)-2-[4-[bis[2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-2,2-dimethyl-4H-1,3-dioxin-4-ylidene]methyl]-3,3'-dihexyl- (9CI) (CA INDEX NAME)

Double bond geometry as described by E or Z.

PAGE 1-A



PAGE 1-B



=> d ibib abs hitstr 2

L56 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:90034 HCAPLUS

DOCUMENT NUMBER: 136:136245

TITLE: Hyperpolarizable organic chromophores

INVENTOR(S): Dalton, Larry R.; Jen, Alex Kwan-Yue; Londergan, Timothy; Carlson, William Brenden; Phelan, Gregory; Huang, Diyun; Casmier, Daniel; Ewy, Todd; Buker, Nicholas

PATENT ASSIGNEE(S): University of Washington, USA

SOURCE: PCT Int. Appl., 104 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

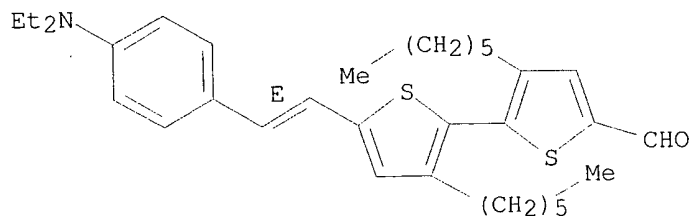
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008215	A1	20020131	WO 2001-US23339	20010724
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002084446	A1	20020704	US 2001-912444	20010724
PRIORITY APPLN. INFO.:			US 2000-220321P	P 20000724
OTHER SOURCE(S):			MARPAT 136:136245	
AB The present invention provides hyperpolarizable org. chromophores based on heterocyclic compds. The chromophores are nonlinear optically active compds. that include a .pi.-donor conjugated to a .pi.-acceptor through a .pi.-electron conjugated bridge. Macromol. structures including the hyperpolarizable org. chromophores are also provided.				
IT 392662-49-6P 392662-52-1P RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prodn. of donor-acceptor conjugated hyperpolarizable heterocyclic org. chromophores)				
RN 392662-49-6 HCAPLUS				
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'--[(1E)-2-[4-(diethylamino)phenyl]ethenyl]-3,3'-dihexyl- (9CI) (CA INDEX NAME)				

Double bond geometry as shown.

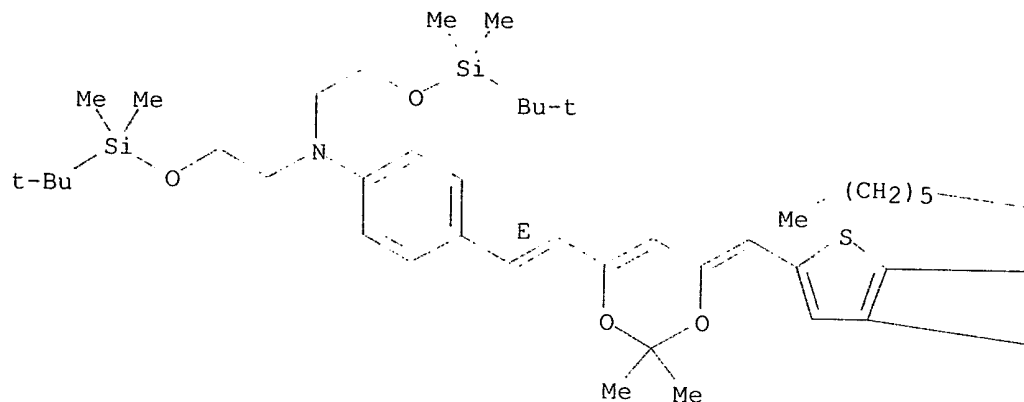


RN 392662-52-1 HCAPLUS

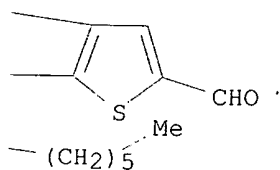
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-[[6-[(1E)-2-[4-[bis[2-[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]amino]phenyl]ethenyl]-2,2-dimethyl-4H-1,3-dioxin-4-ylidene]methyl]-3,3'-dihexyl- (9CI) (CA INDEX NAME)

Double bond geometry as described by E or Z.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

TRAN 09/871,353

see "d que" for L51 for
explanation for
this query display

=> d que 166?

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L1      19 SEA FILE=HCAPLUS ABB=ON PLU=ON CIPRIANI F?/AU
L2      135 SEA FILE=HCAPLUS ABB=ON PLU=ON GIGLI G?/AU
L3      377 SEA FILE=HCAPLUS ABB=ON PLU=ON CINGOLANI R?/AU
L4      48 SEA FILE=HCAPLUS ABB=ON PLU=ON FAVARETTO L?/AU
L5      59 SEA FILE=HCAPLUS ABB=ON PLU=ON ZAMBIANCHI M?/AU
L6      78 SEA FILE=HCAPLUS ABB=ON PLU=ON SOTGIU G?/AU
L7      71 SEA FILE=HCAPLUS ABB=ON PLU=ON CITRO G?/AU
L8      132 SEA FILE=HCAPLUS ABB=ON PLU=ON BARBARELLA G?/AU
L9      734 SEA FILE=HCAPLUS ABB=ON PLU=ON (L1 OR L2 OR L3 OR L4 OR L5
      OR L6 OR L7 OR L8)
L10     54 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 AND THIOPHENE
L11     30 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 AND OLIGOMER?
L12     5 SEA FILE=HCAPLUS ABB=ON PLU=ON L11 AND (THIOPHENE OLIGOMER)/T
      I
L13     24 SEA FILE=REGISTRY ABB=ON PLU=ON (376393-41-8/BI OR 376393-42-
      9/BI OR 376393-43-0/BI OR 376393-44-1/BI OR 492-97-7/BI OR
      111372-97-5/BI OR 111744-23-1/BI OR 113386-74-6/BI OR 116159-99
      -0/BI OR 118347-89-0/BI OR 127236-47-9/BI OR 127236-48-0/BI OR
      127473-73-8/BI OR 127473-74-9/BI OR 127473-75-0/BI OR 139747-07
      -2/BI OR 139747-08-3/BI OR 14762-74-4/BI OR 201604-95-7/BI OR
      201604-98-0/BI OR 25233-34-5/BI OR 376393-45-2/BI OR 5632-29-1/
      BI OR 67984-20-7/BI)
L14     4 SEA FILE=HCAPLUS ABB=ON PLU=ON L12 AND L13
L15     5 SEA FILE=HCAPLUS ABB=ON PLU=ON L12 OR L14
L16     STR

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11

Q
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Hy[^]Hy[^]Hy G1 4 Q[~]C A⁼⁼C Q⁼⁼C⁼⁼N
1 2 3 @5 @6 7 @8 9 10 @12

VAR G1=5/6/8/12/NH2/OH/SH/SO3H/SO2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

GGCAT IS MCY UNS AT 2

GGCAT IS MCY UNS AT 3

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E4 C E1 S AT 1

ECOUNT IS E4 C E1 S AT 2

ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L17 289013 SEA FILE=REGISTRY ABB=ON PLU=ON 16.145.3/RID

L19 STR

Hy[^]Hy[^]Hy
1 2 3

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

GGCAT IS MCY UNS AT 2

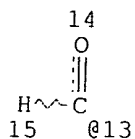
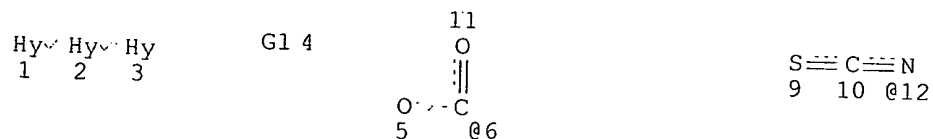
TRAN 09/871,353

GGCAT IS MCY UNS AT 3
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E1 S AT 1
ECOUNT IS E4 C E1 S AT 2
ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

L21 5115 SEA FILE=REGISTRY SUB=L17 SSS FUL L19
L23 2293 SEA,FILE=REGISTRY SUB=L21 SSS FUL L16
L26 STR



VAR G1=OH/SH/NH2/13/6/12

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 5
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY UNS AT 1
GGCAT IS MCY UNS AT 2
GGCAT IS MCY UNS AT 3
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E1 S AT 1
ECOUNT IS E4 C E1 S AT 2
ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L27 1357 SEA FILE=REGISTRY SUB=L23 SSS FUL L26
L28 476 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 3 16.145.3/RID
L29 166 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 4 16.145.3/RID
L30 104 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 5 16.145.3/RID
L31 746 SEA FILE=REGISTRY ABB=ON PLU=ON (L28 OR L29 OR L30)
L32 674 SEA FILE=REGISTRY ABB=ON PLU=ON L31 AND NC=1 NOT ("DIAZO" OR F/ELS)
L33 23948 SEA FILE=REGISTRY ABB=ON PLU=ON 2 16.145.3/RID
L35 2996 SEA FILE=REGISTRY ABB=ON PLU=ON L33 AND "BITHIOPHENE"
L38 662 SEA FILE=REGISTRY ABB=ON PLU=ON L35 AND ("HYDROXY" OR "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORMYL" OR "ISOTHIOCYANATO" OR "THIOL" OR "AMINO" OR "CARBOXYLIC") NOT "ESTER"
L39 584 SEA FILE=REGISTRY ABB=ON PLU=ON L38 AND NC=1
L40 451 SEA FILE=REGISTRY ABB=ON PLU=ON L39 NOT "AZO"
L41 287 SEA FILE=HCAPLUS ABB=ON PLU=ON L32

L42	455	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L40
L43	15	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L41(L)?CONJUGAT?
L44	14	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L42(L)?CONJUGAT?
L45	26	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L43 OR L44
L46	25	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L45 NOT L15
L47	3042811	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	ANTIBOD? OR FLUORESC?(3A)MARKE
					R OR PROTEIN OR DNA OR NUCLEIC OR OLIGONUC? OR HORMON? OR DRUG
					OR MEDICINE OR NEUROTRANSMITTER
L48	121828	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	SPECTROFLUORIMETRY OR
					CYTOMETRY OR FLUORESCENCE(W)MICROSCO? OR GEL ELECTROPHOR?
L49	40	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	(L41 OR L42) AND (L47 OR L48)
L50	8	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L49 AND ?CONJUGAT?
L51	7	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L50 NOT L15
L52	20	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L46 NOT L51
L57	32	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L49 NOT (L50 OR L52)
L60	20	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L57 AND THIOPHEN?/OBI
L61	12	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L57 AND BITHIOPHEN?/OBI
L65	21	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	(L60 OR L61)
L66	2	SEA FILE=HCAPLUS	ABB=ON	PLU=ON	L65 AND (?CONJUGAT? OR LINK?
					OR COVALENT? OR LIGAND)

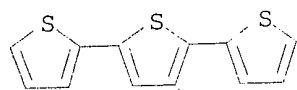
2 cites

=> d ibib abs hitstr 1

L66 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:384558 HCAPLUS
 DOCUMENT NUMBER: 133:28235
 TITLE: Preparation of nanoparticles with polymer shells for use in assays
 INVENTOR(S): Mirkin, Chad A.; Nguyen, Sonbinh T.
 PATENT ASSIGNEE(S): Nanosphere LLC, USA
 SOURCE: PCT Int. Appl., 65 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000033079	A1	20000608	WO 1999-US28387	19991130
W:			AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM	
RW:			GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG	
EP 1135682	A1	20010926	EP 1999-962951	19991130
R:			AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO	
JP 2002531830	T2	20020924	JP 2000-585664	19991130
PRIORITY APPLN. INFO.:			US 1998-110327P P	19981130
			WO 1999-US28387 W	19991130
OTHER SOURCE(S):		MARPAT 133:28235		
AB	The invention provides a method of prepg. nanoparticles having at least one polymer shell attached to them, each polymer shell having a selected property or properties. The method comprises attaching initiation monomers to the surfaces of the nanoparticles, contacting the nanoparticles having the initiation monomers attached to them with a transition metal ring-opening metathesis catalyst to activate the initiation monomers, and contacting the nanoparticles with one or more types of propagation monomers of the formula P-L-N under conditions effective so that the monomers are polymd. to form the one or more polymer shells. In the formula P-L-N, N is a cyclic olefin-contg. group, P is a moiety which gives each polymer shell a selected property or properties, and L is a bond or linker . The invention also provides polymers formed by polymg. the propagation monomers. The invention further provides the nanoparticles, the initiation monomers, and propagation monomers of formula P-L-N wherein P is a moiety having a property selected from the group consisting of redox activity, optical activity, elec. activity and magnetic activity, and L and N are defined above. The invention also provides binding monomers of formula B-L-N, wherein B is a binding moiety that binds specifically to an analyte, and N and L are defined above. Finally, the invention provides methods and kits for detecting or quantitating an analyte.			
IT	273400-09-2, [2,2':5',2''-Terthiophene]-3'-ethanol			
	RL: RCT (Reactant); RACT (Reactant or reagent)			
	(prepn. of nanoparticles with polymer shells for use in assays)			
RN	273400-09-2 HCAPLUS			

CN [2,2':5',2''-Terthiophene]-3'-ethanol (9CI) (CA INDEX NAME)



CH₂-CH₂-OH

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L66 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS
 IC ICM G01N033-553
 ICS B32B005-16
 CC 9-1 (Biochemical Methods)
 Section cross-reference(s): 35
 ST nanoparticle polymer shell assay; binding assay nanoparticle polymer shell; polymn ring opening metathesis polymer shell
 IT Analytical apparatus
 (for binding assays; prepn. of nanoparticles with polymer shells for use in assays)
 IT **Antibodies**
 RL: ARG (Analytical reagent use); TEM (Technical or engineered material use); ANST (Analytical study); USES (Uses)
 (immobilized; prepn. of nanoparticles with polymer shells for use in assays)
 IT Fluorescent substances
 (polymer contg.; prepn. of nanoparticles with polymer shells for use in assays)
 IT **Oligonucleotides**
 RL: ARG (Analytical reagent use); TEM (Technical or engineered material use); ANST (Analytical study); USES (Uses)
 (polymer shell-immobilized; prepn. of nanoparticles with polymer shells for use in assays)
 IT Cycloalkenes
Nucleic acids
 RL: TEM (Technical or engineered material use); USES (Uses)
 (polymer shell-immobilized; prepn. of nanoparticles with polymer shells for use in assays)
 IT Biosensors
 Colorimetry
 Fluorometry
 Nanoparticles
Nucleic acid hybridization
 Redox potential
 Test kits
 (prepn. of nanoparticles with polymer shells for use in assays)
 IT Antigens
 Haptens
Nucleic acids
 RL: ANT (Analyte); ANST (Analytical study)
 (prepn. of nanoparticles with polymer shells for use in assays)
 IT Polymers, preparation
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); TEM (Technical or engineered material use); ANST (Analytical study); PREP

- (Preparation); USES (Uses)
 (prepn. of nanoparticles with polymer shells for use in assays)
- IT Polymerization
 (ring-opening metathesis; prepn. of nanoparticles with polymer shells
 for use in assays)
- IT 220577-97-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (as initiation monomer; prepn. of nanoparticles with polymer shells for
 use in assays)
- IT 220577-87-7P, exo-5-Norbornen-2-yl ferrocenecarboxylate 220577-89-9P,
 exo-5-Norbornen-2-yl ferroceneacetate
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (as propagation monomer; prepn. of nanoparticles with polymer shells
 for use in assays)
- IT 112-55-0, 1-Dodecanethiol
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (in prepn. of gold nanoparticles capped with linear alkanethiols;
 prepn. of nanoparticles with polymer shells for use in assays)
- IT 7440-57-5, Gold, uses
 RL: TEM (Technical or engineered material use); USES (Uses)
 (nanoparticles; prepn. of nanoparticles with polymer shells for use in
 assays)
- IT 172222-30-9
 RL: CAT (Catalyst use); USES (Uses)
 (prepn. of nanoparticles with polymer shells for use in assays)
- IT 220577-91-3DP, gold nanoparticle-immobilized 220577-93-5DP, gold
 nanoparticle-immobilized 273400-11-6P 273400-13-8P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of nanoparticles with polymer shells for use in assays)
- IT 79-37-8, Oxalyl chloride 124-41-4, Sodium methoxide 623-24-5
 1271-42-7, Ferrocenecarboxylic acid 1271-86-9, N,N-
 Dimethylaminomethylferrocene 1287-16-7, Ferroceneacetic acid
 2321-07-5, Fluorescein 2890-98-4, exo-5-Norbornen-2-ol 5257-37-4
 5713-61-1, (2-Thienyl)magnesiumbromide 6964-21-2, 3-
Thiopheneacetic acid 7087-68-5, N, N-Diisopropylethylamine
 10387-40-3, Potassium thioacetate 13191-37-2 42758-92-9 66605-79-6,
 10-Chlorodecyl toluene-4 sulfonate 72287-26-4 89992-70-1
 273400-09-2, [2,2':5',2''-Terthiophene]-3'-ethanol 273400-12-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of nanoparticles with polymer shells for use in assays)
- IT 220577-95-7P 220577-99-1P 273400-05-8P 273400-07-0P 273400-14-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. of nanoparticles with polymer shells for use in assays)
- IT 220577-91-3P 273400-06-9P 273400-08-1P 273400-10-5P 273400-15-0P
 273400-16-1P 273400-17-2P 273932-27-7P 273932-30-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of nanoparticles with polymer shells for use in assays)
- IT 50-99-7D, D-Glucose, polymer shell-immobilized, uses 69-79-4D, Maltose,
 polymer shell-immobilized 99685-96-8D, Fullerene-C60, polymer
 shell-immobilized
 RL: TEM (Technical or engineered material use); USES (Uses)
 (prepn. of nanoparticles with polymer shells for use in assays)
- IT 16903-35-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (redn. of, in prepn. of gold nanoparticles capped with linear
 alkanethiols; prepn. of nanoparticles with polymer shells for use in
 assays)

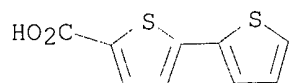
TRAN 09/871,353

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L66 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1998:709262 HCAPLUS
 DOCUMENT NUMBER: 129:326078
 TITLE: Use of one-dimensional nuclear magnetic resonance to
 identify ligands to target biomolecules
 INVENTOR(S): Fesik, Stephen W.; Hajduk, Philip J.; Olejniczak,
 Edward T.
 PATENT ASSIGNEE(S): Abbott Laboratories, USA
 SOURCE: PCT Int. Appl., 28 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9848264	A1	19981029	WO 1998-US7907	19980417
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 6043024	A	20000328	US 1997-844124	19970418
ZA 9802919	A	19981012	ZA 1998-2919	19980406
AU 9871380	A1	19981113	AU 1998-71380	19980417
EP 975954	A1	20000202	EP 1998-918461	19980417
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI, RO				
BR 9808079	A	20000308	BR 1998-8079	19980417
JP 2002507277	T2	20020305	JP 1998-546228	19980417
NO 9905078	A	19991206	NO 1999-5078	19991018
PRIORITY APPLN. INFO.: US 1997-844124 A 19970418				
WO 1998-US7907 W 19980417				
AB	The invention provides a process for identifying compds. which bind to a specific target mol. (protein , receptor, nucleic acid , etc.). The process comprises (a) generating a 1st T2- or diffusion-filtered proton spectrum of 1 or a mixt. of chem. compds.; (b) exposing 1 or a mixt. of chem. compds. to the target mol.; (c) generating a 2nd T2- or diffusion-filtered proton spectrum of 1 or a mixt. of chem. compds. that has been exposed to the target mol. in step (b); and (d) comparing the 1st and 2nd T2- or diffusion-filtered proton spectra to det. differences between the 1st and the 2nd spectra, the differences identifying the presence of .gtoreq.1 compds. that are ligands which have bound to the target mol.			
IT	2060-55-1, [2,2'- Bithiophene]-5-carboxylic acid RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process) (one-dimensional T2- or diffusion-filtered NMR to identify ligands to target biomols.)			
RN	2060-55-1 HCAPLUS			
CN	[2,2'-Bithiophene]-5-carboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)			

TRAN 09/871,353



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

see the dque for L51
for an explanation
of this query
display

=> d que 171

L16

STR

11

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Hy Hy Hy G1 4 Q -C A=C Q=C=N
1 2 3 @5 @6 7 @8 9 10 @12

VAR G1=5/6/8/12/NH2/OH/SH/SO3H/SO2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

GGCAT IS MCY UNS AT 2

GGCAT IS MCY UNS AT 3

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E4 C E1 S AT 1

ECOUNT IS E4 C E1 S AT 2

ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L17 289013 SEA FILE=REGISTRY ABB=ON PLU=ON 16.145.3/RID
L19 STR

Hy^Hy^Hy
1 2 3

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

GGCAT IS MCY UNS AT 2

GGCAT IS MCY UNS AT 3

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E4 C E1 S AT 1

ECOUNT IS E4 C E1 S AT 2

ECOUNT IS E4 C E1 S AT 3

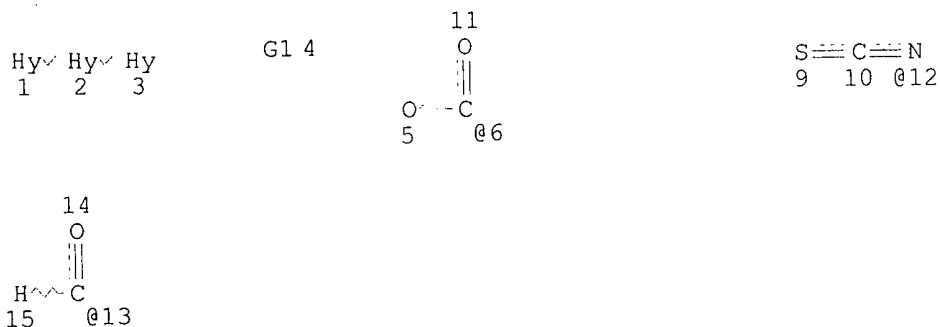
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

L21 5115 SEA FILE=REGISTRY SUB=L17 SSS FUL L19
L23 2293 SEA FILE=REGISTRY SUB=L21 SSS FUL L16
L26 STR



VAR G1=OH/SH/NH2/13/6/12

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 5
 DEFAULT MLEVEL IS ATOM
 GGCAT IS MCY UNS AT 1
 GGCAT IS MCY UNS AT 2
 GGCAT IS MCY UNS AT 3
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS E4 C E1 S AT 1
 ECOUNT IS E4 C E1 S AT 2
 ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L27 1357 SEA FILE=REGISTRY SUB=L23 SSS FUL L26
 L28 476 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 3 16.145.3/RID
 L29 166 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 4 16.145.3/RID
 L30 104 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 5 16.145.3/RID
 L31 746 SEA FILE=REGISTRY ABB=ON PLU=ON (L28 OR L29 OR L30)
 L32 674 SEA FILE=REGISTRY ABB=ON PLU=ON L31 AND NC=1 NOT ("DIAZO" OR F/ELS)
 L33 23948 SEA FILE=REGISTRY ABB=ON PLU=ON 2 16.145.3/RID
 L35 2996 SEA FILE=REGISTRY ABB=ON PLU=ON L33 AND "BITHIOPHENE"
 L38 662 SEA FILE=REGISTRY ABB=ON PLU=ON L35 AND ("HYDROXY" OR "HYDROXYL" OR "CARBOXALDEHYDE" OR "FORMYL" OR "ISOTHIOCYANATO" OR "THIOL" OR "AMINO" OR "CARBOXYLIC") NOT "ESTER"
 L39 584 SEA FILE=REGISTRY ABB=ON PLU=ON L38 AND NC=1
 L40 451 SEA FILE=REGISTRY ABB=ON PLU=ON L39 NOT "AZO"
 L41 287 SEA FILE=HCAPLUS ABB=ON PLU=ON L32
 L42 455 SEA FILE=HCAPLUS ABB=ON PLU=ON L40
 L43 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L41(L)?CONJUGAT?
 L44 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L42(L)?CONJUGAT?
 L45 26 SEA FILE=HCAPLUS ABB=ON PLU=ON L43 OR L44
 L67 57 SEA FILE=HCAPLUS ABB=ON PLU=ON (L41 OR L42) AND (VISIBLE(3A)(UV OR ULTRAVIOLET))
 L68 52 SEA FILE=HCAPLUS ABB=ON PLU=ON L67 NOT (L43 OR L45)
 L69 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L68 AND (?CONJUGAT? OR LINK? OR COVALENT? OR LIGAND)
 L70 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L69 NOT PATENT/DT
 L71 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L70 AND PD<20010530

14 cites

=> d ibib abs hitstr 1-14

L71 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:755282 HCAPLUS

DOCUMENT NUMBER: 136:207032

TITLE: Spectral characteristics of bithiophenes and terthiophenes linked with heterocyclic unit in solution and polymer matrix

AUTHOR(S): Hrdlovic, Pavol; Krajcovic, Jozef; Vegh, Daniel
CORPORATE SOURCE: Polymer Institute, Slovak Academy of Sciences, Bratislava, 842 36, SlovakiaSOURCE: Journal of Photochemistry and Photobiology, A: Chemistry (2001), 144(2-3), 73-82
CODEN: JPPCEJ; ISSN: 1010-6030

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

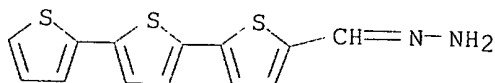
LANGUAGE: English

AB Spectral characteristics of derivs. of thiophene substituted on heteroarom. cycle as pyrazine was compared with terthiophene linked with cyano- and hydrazo groups. The absorption, fluorescence and its lifetime were measured in soln. (methanol, cyclohexane) and in polymer matrixes (polystyrene, PS; PMMA; and poly(vinyl chloride) (PVC)). Derivs. with two thiophene units substitute on pyrazine exhibit the lowest wavenumber band in the region 26,320-25,600 cm⁻¹ and log .vepsiln. .apprx.4.0, which is not influenced by the medium. Derivs. with benzene and pyridine ring annealed to pyrazine (2,3-bis-(2'-thienyl)quinoxaline (I), 2,3-bis-(2'-thienyl)pyrido[2,3-b]pyrazine (III)) exhibit fluorescence in polar methanol with max. at 22,200 cm⁻¹ and quantum yield of about 0.2 which is blue-shifted in going to non-polar solvent. The max. fluorescence is slightly blue-shifted in polymer matrixes as compared to methanol. Derivs. with annealed thiophene to pyrazine or substituted with two cyano groups (2,3-bis-(2'-thienyl)thieno[3,4-b]pyrazine (II), 2,3-dicyano-5,6-bis(2'-thienyl)pyrazine (IV)) do not yield any emission. Derivs. with terthiophene structural units ([2,2',5',2'']-terthiophene-[2]-thienylacrylonitrile (V) [2,2',5',2'']-terthiophene-5-carbaldehydehydrazone (VI)) exhibit fluorescence with max. around 20,000 cm⁻¹. The lifetime of fluorescence of all thiophene was 1 ns or shorter. The polymer matrixes increase the intensity of fluorescence to some extent and prolong the lifetime of thiophene derivs. Deriv. VI exhibits some tendency to an aggregation at higher concn. above 0.01 mol kg⁻¹ in polymer matrixes.

IT 188123-63-9P, [2,2',5',2'']-Terthiophene-5-carbaldehydehydrazone
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(optical absorption and emission and lifetime of emission of bis-thiophenes and ter-thiophenes linked by heterocyclic unit studied in solns. and in polymer matrixes)

RN 188123-63-9 HCAPLUS

CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde, hydrazone (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:313940 HCAPLUS

DOCUMENT NUMBER: 135:161594

TITLE: Electronic and magnetic metal-metal interactions in dinuclear oxomolybdenum(V) complexes across bis-phenolate bridging **ligands** with different spacers between the phenolate termini: **ligand**-centered vs. metal-centered redox activity

AUTHOR(S): Bayly, Simon R.; Humphrey, Elizabeth R.; de Chair, Helena; Paredes, Cecilia G.; Bell, Zoe R.; Jeffery, John C.; McCleverty, Jon A.; Ward, Michael D.; Totti, Federico; Gatteschi, Dante; Courric, Stephane; Steele, Barry R.; Screttas, Constantinos G.

CORPORATE SOURCE: School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK

SOURCE: Journal of the Chemical Society, Dalton Transactions (2001), (9), 1401-1414
CODEN: JCSDAA; ISSN: 1472-7773

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

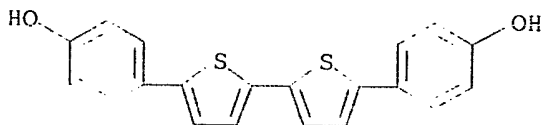
AB Dinuclear complexes were prep'd. in which two {MoV(TpMe,Me)(O)Cl} fragments (abbreviated as Mo; TpMe,Me = tris(3,5-dimethylpyrazol-1-yl)hydroborate) are attached to either end of a bis-p-phenolate bridging **ligand** [(4,4'-OC₆H₄)-X-(4,4'-C₆H₄O)]₂-. The complexes are Mo₂(C:C) (X = CH:CH), Mo₂(C:C)₂ (X = CH:CH-CH:CH), Mo₂(C:C)₃ (X = CH:CH-CH:CH-CH:CH), Mo₂(th) (X = 2,5-thiophenediyl), Mo₂(th)₂ (X = 2,5:2',5'-bithiophenediyl), Mo₂(th)₃ (X = 2,5:2',5':2'',5''-terthiophenediyl), Mo₂(C.tplbond.C) (X = C.tplbond.C), Mo₂(N:N) (X = N:N), Mo₂(CO) [X = C(O)] and Mo₂(C₂.PHI.C₂) [X = CH:CH(1,4-C₆H₄)CH:CH]. Electrochem., UV/visible/NIR spectroelectrochem. and magnetic measurements were carried out to see how effectively the different spacer groups X mediate electronic and magnetic interactions between the two redox-active, paramagnetic, Mo centers. The electronic interactions were det'd. from the redox sepn. between the two successive 1-electron oxidns. which are formally Mo(VI)-Mo(V) couples; thienyl units in the bridging **ligand** are much more effective at maintaining electronic communication over long distances than p-phenylene or ethenyl spacers of comparable lengths. The azo (N:N) **linkage** afforded a much weaker electronic interaction than the ethenyl or ethynyl spacers. UV/visible/NIR spectroelectrochem. studies showed that whereas the 1st oxidn. is metal-centered to give Mo(VI)-Mo(V) species with characteristic intense phenolate Mo(VI) LMCT transitions in the near-IR region, the spectra of the doubly oxidized complexes are characteristic of quinones: thus, the sequence of species formed on oxidn. is [Mo(V)(.mu.-diolate)Mo(V)]₀.fwdarw. [Mo(V)(.mu.-diolate)Mo(VI)]₊.fwdarw. [Mo(V)(.mu.-quinone)Mo(V)]₂₊, with an internal charge redistribution assoc'd. with the 2nd oxidn. Semi-empirical ZINDO calcs. provide some support for this. Magnetic susceptibility measurements on Mo₂(C:C), Mo₂(th), Mo₂(N:N) and Mo₂(C.tplbond.C) show that all are weakly antiferromagnetically coupled, as expected from a spin-polarization picture, with the order of strength of the magnetic interaction being the reverse of the order for electronic coupling, such that Mo₂(th) affords the strongest electronic interaction but the weakest magnetic interaction.

IT 185413-64-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for prepn. of oxomolybdenum(V) tris(dimethylpyrazolyl)hydroborato chloro dinuclear complex bridged by bis-phenolato **ligand**)

RN 185413-64-3 HCAPLUS

CN Phenol, 4,4'-[2,2'-bithiophene]-5,5'-diylbis- (9CI) (CA INDEX NAME)

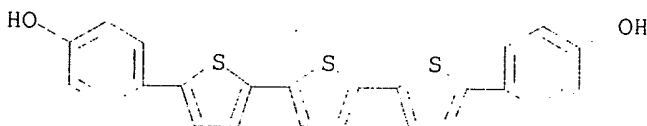


IT 352462-92-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reactant for prepn. of oxomolybdenum(V) tris(dimethylpyrazolyl)hydroborato chloro dinuclear complex bridged by bis-phenolato ligand)

RN 352462-92-1 HCAPLUS

CN Phenol, 4,4'-[2,2':5',2''-terthiophene]-5,5''-diylbis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 96 THERE ARE 96 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:367325 HCAPLUS

DOCUMENT NUMBER: 133:73758

TITLE: Photoinduced Energy and Electron Transfer in Fullerene-Oligothiophene-Fullerene Triads

AUTHOR(S): Van Hal, Paul A.; Knol, Joop; Langeveld-Voss, Bea M. W.; Meskers, Stefan C. J.; Hummelen, J. C.; Janssen, Rene A. J.

CORPORATE SOURCE: Laboratory of Macromolecular and Organic Chemistry, Eindhoven University of Technology, Eindhoven, 5600 MB, Neth.

SOURCE: Journal of Physical Chemistry A (2000), 104(25), 5974-5988

CODEN: JPCAFH; ISSN: 1089-5639

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of fullerene-oligothiophene-fullerene (C60-nT-C60) triads with n = 3, 6, or 9 thiophene units has been synthesized, and their photophys. properties have been studied using photoinduced absorption and fluorescence spectroscopy in soln. and in the solid state as thin films. The results are compared to those of mixts. of oligothiophenes (nT) with N-methylfulleropyrrolidine (MP-C60). Photoexcitation of the triads in the film results in an electron-transfer reaction for n = 6 and 9, but not for n = 3. The lifetime of the charge-sepd. state in the film is on the order of milliseconds. Photoexcitation of the oligothiophene moiety of the C60-nT-C60 triads, dissolved in an apolar solvent, results in a singlet energy-transfer reaction to the fullerene moiety with rates varying between 10¹² and 10¹³ s⁻¹. In more polar solvents, an intramol.

photoinduced charge sepn. occurs for $n = 6$ and 9 and, to some extent, for $n = 3$. The quenching of the MP-C60(S1) fluorescence provides a lower limit to the rate of the intramol. photoinduced electron transfer of 10^{11} s $^{-1}$ in the C60-nT-C60 triads with $n = 6$ or 9 in polar solvents, assuming that charge sepn. occurs after singlet energy transfer from nT(S1) to MP-C60(S1). A direct mechanism, i.e., charge sepn. from nT(S1), cannot be excluded exptl. but must occur in the femtosecond time domain to compete effectively with energy transfer. The lifetime of the intramolecularly charge-sepd. state in the C60-nT-C60 triads is significantly reduced compared to the lifetime of the radical ions in the films, and hence, the latter results from charge migration to different mol. sites. Similar energy- and electron-transfer reactions occur intermolecularly in soln. from the nT and MP-C60 triplet states. The preferences for intra- and intermol. energy- and electron-transfer reactions, as a function of **conjugation** length and solvent permittivity, are in full agreement with predictions that can be made using the Weller equation for the change in free energy upon charge sepn.

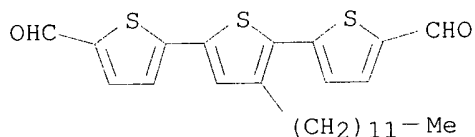
IT 252684-40-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(Prato reaction in regioisomer mixt.; photoinduced energy and electron transfer in fullerene-oligothiophene-fullerene triads)

RN 252684-40-5 HCAPLUS

CN [2,2':5',2''-Terthiophene]-5,5''-dicarboxaldehyde, 3'-dodecyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 103 THERE ARE 103 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:712697 HCAPLUS

DOCUMENT NUMBER: 132:64385

TITLE: Ferrocene End-Capped Palladium(II) and Platinum(II) Complexes with Thiophene Spacers

AUTHOR(S): Thomas, K. R. Justin; Lin, Jiann T.; Lin, Kuan-Jiuh

CORPORATE SOURCE: Institute of Chemistry, Academia Sinica, Taipei, 115, Taiwan

SOURCE: Organometallics (1999), 18(25), 5285-5291

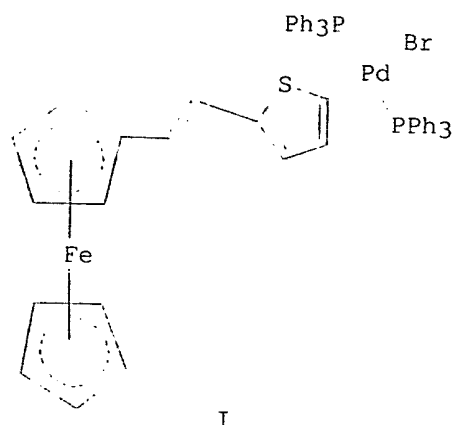
CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

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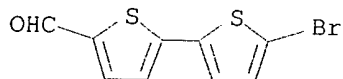


AB Heterobimetallics contg. ferrocene and Pd(II) or Pt(II), e.g., I, were synthesized by oxidative addn. of ferrocene-substituted halothiophenes with zerovalent Pd or Pt precursors. The stable solids were thoroughly characterized by elemental anal., NMR, **UV-visible** spectroscopy, and cyclic voltammetry. The rich redox chem. of the complexes depends on the **conjugation** length that separates the two metal sites. The crystal structure of a Pt .sigma.-thienyl complex I was detd.

IT 110046-60-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Wittig reaction with (ferrocenylmethyl)triphenylphosphonium bromide)

RN 110046-60-1 HCAPLUS

CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-bromo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:305626 HCAPLUS

DOCUMENT NUMBER: 131:58548

TITLE: Intramolecular energy transfer of [60]fullerene-linked oligothiophenes

AUTHOR(S): Yamashiro, Takashi; Aso, Yoshio; Otsubo, Tetsuo; Tang, Heqing; Harima, Yutaka; Yamashita, Kazuo

CORPORATE SOURCE: Faculty of Engineering, Hiroshima University, Higashi-Hiroshima, 739-8527, Japan

SOURCE: Chemistry Letters (1999), (5), 443-444

CODEN: CMLTAG; ISSN: 0366-7022

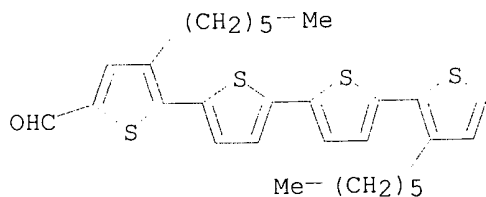
PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB [60]Fullerene-linked quarter-, octi-, and duodecithiophenes have been synthesized, and their emission spectra demonstrate efficient intramol. energy transfer from the thiophene moiety to the fullerene, whose rate const. largely depends on the chain length of the

oligothiophene moiety.
 IT 228414-99-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. of [60]fullerene-linked oligothiophenes and
 chain-length dependence of their intramol. energy transfer assessed
 from fluorescence quenching measurements)
 RN 228414-99-1 HCAPLUS
 CN [2,2':5',2'':5'',2'''-Quaterthiophene]-5-carboxaldehyde, 3,3'''-dihexyl-
 (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1998:786650 HCAPLUS
 DOCUMENT NUMBER: 130:139711
 TITLE: A Novel Series of p-n Diblock Light-Emitting Copolymers Based on Oligothiophenes and 1,4-Bis(oxadiazolyl)-2,5-dialkyloxybenzene
 AUTHOR(S): Huang, Wei; Meng, Hong; Yu, Wang-Lin; Pei, Jian; Chen, Zhi-Kuan; Lai, Yee-Hing
 CORPORATE SOURCE: Institute of Materials Research and Engineering and Department of Chemistry, National University of Singapore, Singapore, 119260, Singapore
 SOURCE: Macromolecules (1999), 32(1), 118-126
 CODEN: MAMOBX; ISSN: 0024-9297
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A new series of p-n diblock **conjugated** copolymers consisting of alternate 1,4-bis(oxadiazolyl)-2,5-dialkyloxybenzene and oligothiophenes with one to three thiophene rings (P1-P3) have been synthesized. The polymers have well-defined structures and exhibit good thermal stability with the onset decompn. temps. in nitrogen at around 300 .degree.C. The glass transition temp. (Tg) of the polymers decreases with increasing the length of oligothiophene blocks. Both the absorption spectra and photoluminescence spectra shift to longer wavelength with increase in the length of oligothiophene blocks. The emissive color of the polymers could be tuned from blue to green to orange just by increasing the no. of thiophene rings in the oligothiophene blocks from one to three. No obvious change in redn. potential is found for the polymers with variation in the length of oligothiophene blocks. The redn. potential E1/2 of the polymers is measured by cyclic voltammetry to be around -1.7 V vs SCE, comparable to those of poly(cyanoterephthalidene) (CN-PPV) and other good electron-transporting materials. The oxidn. potential of the polymers can be reduced remarkably by increasing the length of oligothiophene blocks. The oxidn. potential E1/2 of P3 is measured to be 1.25 V with the onset potential at 1.0 V vs SCE. These values are comparable to those of some hole-injection favorable electroluminescent polymers. The results prove

that the p-n diblock structure may be a promising mol. design for synthetically tuning the HOMO and LUMO of **conjugated** polymers.

IT 215324-18-8P

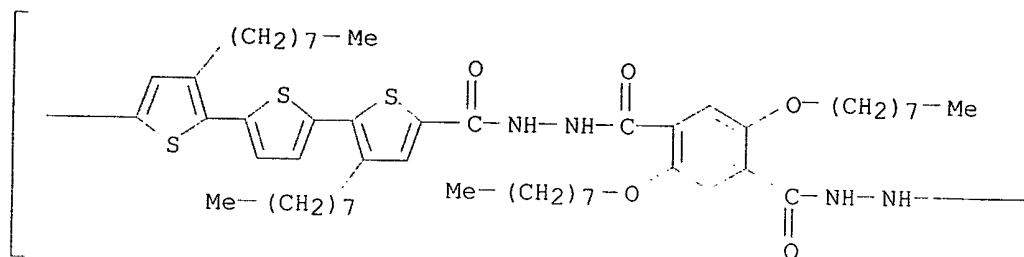
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and physicochem. properties of series of light-emitting copolymers based on oligothiophenes and 1,4-bis(oxadiazolyl)-2,5-dialkyloxybenzene)

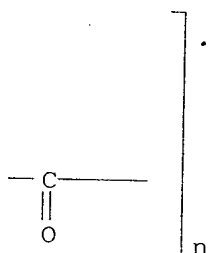
RN 215324-18-8 HCAPLUS

CN Poly[(3,3''-dioctyl[2,2':5',2''-terthiophene]-5,5''-diyl)carbonylhydrazocarbonyl[2,5-bis(octyloxy)-1,4-phenylene]carbonylhydrazocarbonyl] (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



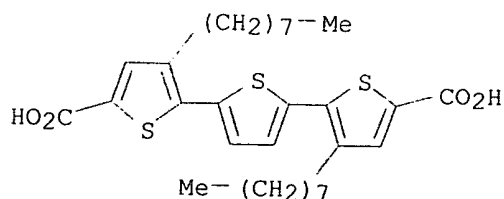
IT 216772-47-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(reactant in monomer prepn.; prepn. and physicochem. properties of series of light-emitting copolymers based on oligothiophenes and 1,4-bis(oxadiazolyl)-2,5-dialkyloxybenzene)

RN 216772-47-3 HCAPLUS

CN [2,2':5',2''-Terthiophene]-5,5''-dicarboxylic acid, 3,3''-dioctyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:786594 HCAPLUS

DOCUMENT NUMBER: 130:102060

TITLE: Adsorption of Carboxyl-Terminated Dithiophene and Terthiophene Molecules on ITO Electrodes and Their Electrochemical Coupling to Polymer Layers. The Influence of Molecular Geometry

AUTHOR(S): Berlin, Anna; Zotti, Gianni; Schiavon, Gilberto; Zecchin, Sandro

CORPORATE, SOURCE: Centro CNR di Sintesi e Stereochimica di Speciali Sistemi Organici, Milan, 20133, Italy

SOURCE: Journal of the American Chemical Society (1998

), 120(51), 13453-13460

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Carboxypentyl and carboxyhexyl bithiophenes and terthiophenes, in which the oligothiophene tail is either perpendicularly or linearly **linked** to the tethering carboxyalkyl chain, were adsorbed on ITO electrodes. The obtained stable monolayers are anodically oxidized in acetonitrile to produce polymer layers (storing a reversible charge of 15 .mu.C cm⁻²) in the case of perpendicular adsorbates whereas linear bithiophene and terthiophene are able to couple only with oligothiophenes in soln. Electrochem. and **UV-visible** spectroscopic anal. indicate that the polymer layers are in fact constituted by thiophene hexamers. The adsorbed linear terthiophene may be coupled with the terthiophene itself in soln. to produce a 1-end surface-grafted sexithiophene monolayer (reversible charge 40 .mu.C cm⁻²), whereas a two-end surface-grafted sexithiophene with the same coverage is produced by adsorption of the .alpha.-coupled terthiophene. The 1-end and two-end grafted sexithiophene monolayers display different electrochem. and spectral patterns. Chronoamperometry and cyclic voltammetry show that the adsorbed linear bithiophene may be oxidatively coupled with 2,2'-bithiophene in soln. to produce surface-anchored polythiophene chains.

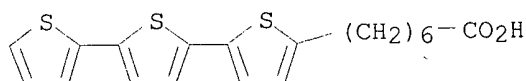
IT 219535-15-6P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(prepn. and adsorption of carboxyl-terminated dithiophene and terthiophene mols. on ITO electrodes and electrochem. coupling to polymer layers: influence of mol. geometry)

RN 219535-15-6 HCAPLUS

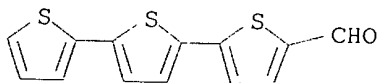
CN [2,2':5',2''-Terthiophene]-5-heptanoic acid (9CI) (CA INDEX NAME)



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:752380 HCAPLUS
 DOCUMENT NUMBER: 130:167979
 TITLE: Investigation of exciton coupling in oligothiophenes by circular dichroism spectroscopy
 AUTHOR(S): Langeveld-Voss, Bea M. W.; Beljonne, David; Shuai, Zhigang; Janssen, Rene A. J.; Meskers, Stefan C. J.; Meijer, E. W.; Bredas, Jean-Luc
 CORPORATE SOURCE: Lab. Macromolecular Organic Chemistry, Eindhoven Univ. Technology, Eindhoven, 5600 MB, Neth.
 SOURCE: Advanced Materials (Weinheim, Germany) (1998), 10(16), 1343-1348
 CODEN: ADVMEW; ISSN: 0935-9648
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB To study the effect of exciton coupling on thiophene chromophores, the model compds. N,N'-bis([2,2';5',2'']terthiophen-5''-ylmethylene)cyclohexane-(1S,2S)-diamine (I) and (1R-phenylethyl)-[2,2';5',2'']terthiophen-5''-ylmethylene amine were prepd. and characterized by UV, CD, and fluorescence spectroscopy which were also theor. simulated. The bisignate CD spectrum of I resulted from a right-handed chiral orientation of the 2 terthienyl units with respect to each other. The exciton coupling in I was .apprxeq.0.15-0.2 eV. These observations were consistent with the explanation that the bisignate CD spectra in .pi.-conjugated polymers with optically active pendant side chains were caused by a chiral superstructure of predominantly planar chains. Since the CD spectra of I and those of optically active conjugated polymers looked alike, it was assumed that the exciton coupling should be of the same order of magnitude.
 IT 7342-41-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of oligothiophenes and their exciton coupling studied by CD)
 RN 7342-41-8 HCAPLUS
 CN [2,2':5',2'']-Terthiophene]-5-carboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1998:186798 HCAPLUS
 DOCUMENT NUMBER: 128:167880
 TITLE: Alternating Conjugated and Nonconjugated Polymer. 1. Crystal Structures and Polymorphism of Poly(hexamethylene 2,2,-bithiophene-5,5,-dicarboxylate), P6BT
 AUTHOR(S): Wang, Shanger; Brisse, Francois
 CORPORATE SOURCE: Departement de Chimie, Universite de Montreal, Montreal, QC, H3C 3J7, Can.
 SOURCE: Macromolecules (1998), 31(7), 2265-2277
 CODEN: MAMOBX; ISSN: 0024-9297
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal

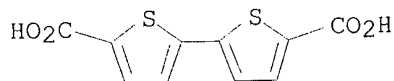
LANGUAGE:

English

AB X-ray fiber diffraction and DSC investigations of the title polymer, P6BT, reveal the existence of three polymorphs. Both .alpha.- and .beta.-forms belong to the monoclinic system, while in the .gamma.-form, the chains are packed in a triclinic unit cell. In all three forms the bithiophenedicarboxylate group is confined in a .pi.-conjugated plane; however, with different orientations of the carbonyl group relative to the sulfur atom (in .alpha.- and .beta.-forms, S-C-C:O is in the cis conformation, while in the .gamma.-form, S-C-C:O is trans). The methylenic sequence in the .beta.- and .gamma.-forms is in the all-trans conformation with only slight deviations from planarity. With a torsion (.tau.3) around the C-O bond between the arom. plane and aliph. segment, the polymer chain changes its overall shape from ribbonlike in the .alpha.-form (.tau.3 .apprx. 180.degree.) to a sine-curve shape in the .beta.-form (.tau.3 = 173.degree.) and finally to a zigzag in the .gamma.-form (.tau.3 = 103.degree.). The .alpha.-form is paracryst., with random displacements of the chains along the fiber axis. The four chains in the unit cell of the .beta.-form are found in two pairs displaced by 5.63 .ANG. from each other, in the c-axis direction. Within the pair, the chains adopt an antiparallel disposition. The arom. planes are arranged nearly parallel to the ac plane in a "side-by-side" pattern in the a-direction. Chains in the .gamma.-form pack in successive layers, where the bithiophene dicarboxylic planes aggregate in a "face-to-face" fashion, forming well-organized .pi.-stacks favorable for the interchain charge transfer of the alternating **conjugated** and **nonconjugated** polymer. The interplanar distance between neighboring bithiophene planes is 3.56 .ANG.. The chain conformation and crystal packing in the .gamma.-form resemble those obsd. in the model compd., di-n-hexyl 2,2'-bithiophene-5,5'-dicarboxylate (6BT6). A monotropic mesophase with unique chain arrangements was found to occur during heating. The transformation temps. are as follows: .alpha.- to .beta.-form, 130-150 .degree.C; .beta.- to .gamma.-form, 161 .degree.C; .gamma.-form to mesophase, 172 .degree.C; and mesophase to isotropic liq., around 185 .degree.C. The strong .pi.-.pi. interaction between arom. planes is believed to be the main driving force of the phase transformations. Due to this solid-state ordering process, the bathochromic shift in the **UV-visible** region was obsd. Some abnormal phenomena such as preferred tilt of crystal in the .gamma.-form are described. The relationship between these structures and those of the biphenyl analog, poly(hexamethylene 4,4'-biphenyldicarboxylate) are discussed.

IT **3515-34-2P**, 2,2'-Bithiophene-5,5'-dicarboxylic acid
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (crystal structures and polymorphism of poly(hexamethylene 2,2'-bithiophene-5,5'-dicarboxylate))

RN 3515-34-2 HCAPLUS
 CN [2,2'-Bithiophene]-5,5'-dicarboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



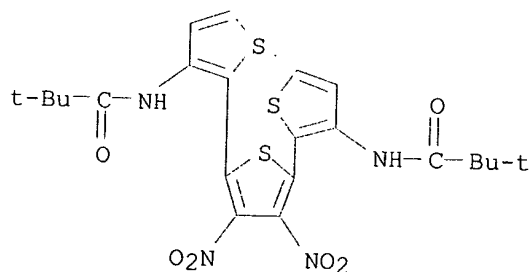
L71 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1997:324841 HCAPLUS
 DOCUMENT NUMBER: 127:34576
 TITLE: Low Optical Bandgap Polythiophenes by an Alternating

AUTHOR(S): Donor/Acceptor Repeat Unit Strategy
 Zhang, Qing; Tour, James M.
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, University
 of South Carolina, Columbia, SC, 29208, USA
 SOURCE: Journal of the American Chemical Society (1997
), 119(21), 5065-5066
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

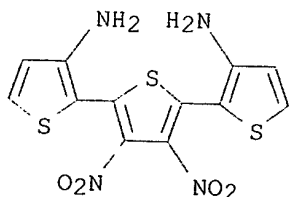
AB This paper describes a method to increase delocalization between consecutive repeat units in **conjugated** polymers by constructing alternating step growth [AB] polymers where the A-units are electron rich and the B-units are electron deficient. The low optical bandgap polymers based on polythiophenes are prep'd. by a modified Stille polymn. using a Pd(0) and CuI pre-catalyst system in which aryl dibromides couple with aryl distannanes. The donor units are 3,4-diaminothiophene or an N,N'-bis(tert-butoxycarbonyl)-3,4-diaminothiophene, and the acceptor units are 3,4-dinitrothiophene or a 3,4-n-butylimidothiophene. The optical spectra show λ_{max} values ranging from 526-662 nm, consistent with a decrease in the bandgap. The nitro-contg. polymer is only sol. in polar solvents such as methanol, DMSO, and water, suggesting significant zwitterionic character. Several model trimers were prep'd. which have significantly shorter wavelength optical absorptions, thus confirming the need for the extended polymeric systems.

IT 190723-21-8 190723-23-0
 RL: PRP (Properties)
 (model comp'd.; prepn. of low optical bandgap polythiophenes by an alternating donor-acceptor repeat unit strategy)

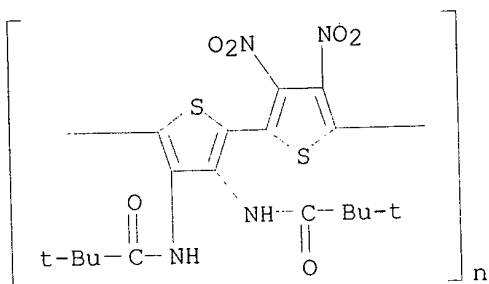
RN 190723-21-8 HCAPLUS
 CN Propanamide, N,N'-(3',4'-dinitro[2,2':5',2''-terthiophene]-3,3''-diyl)bis[2,2'-dimethyl- (9CI) (CA INDEX NAME)



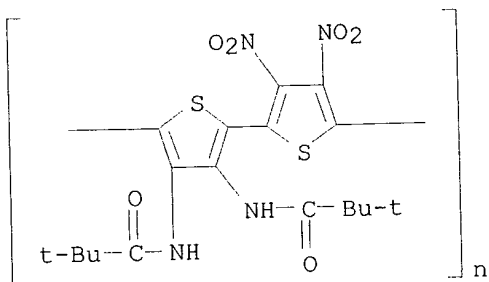
RN 190723-23-0 HCAPLUS
 CN [2,2':5',2''-Terthiophene]-3,3''-diamine, 3',4'-dinitro- (9CI) (CA INDEX NAME)



IT 190723-08-1P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of low optical bandgap polythiophenes by an alternating donor-acceptor repeat unit strategy)
 RN 190723-08-1 HCAPLUS
 CN Poly[3,4-bis[(2,2-dimethyl-1-oxopropyl)amino]-3',4'-dinitro[2,2'-bithiophene]-5,5'-diyl] (9CI) (CA INDEX NAME)



IT 190723-08-1DP, deprotected
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of low optical bandgap polythiophenes by an alternating donor-acceptor repeat unit strategy)
 RN 190723-08-1 HCAPLUS
 CN Poly[3,4-bis[(2,2-dimethyl-1-oxopropyl)amino]-3',4'-dinitro[2,2'-bithiophene]-5,5'-diyl] (9CI) (CA INDEX NAME)



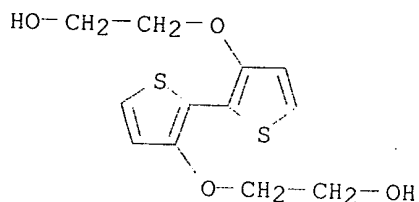
L71 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1995:797754 HCAPLUS
 DOCUMENT NUMBER: 123:352978
 TITLE: Ionoresistivity as a highly sensitive sensory probe: investigations of polythiophenes functionalized with calix[4]arene-based ion receptors
 AUTHOR(S): Marsella, Michael J.; Newland, Robert J.; Carroll, Patrick J.; Swager, Timothy M.
 CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104-6323, USA
 SOURCE: Journal of the American Chemical Society (1995), 117(39), 9842-8
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The authors report the synthesis, optical, and electrochem. properties of a calix[4]arene-substituted polythiophene which demonstrates ion-selective voltammetric, chromic, fluorescent, and resistive responses. The ionochromic response of this polythiophene on exposure to Na⁺ shows an increased effective conjugation length of the polymer backbone. Despite this, Na⁺ induces a large pos. shift in the potential at which the polymer is oxidized (greater than +100 mV) commensurate with a large decrease in cond. (>99%). Although the calix[4]arene-substituted polythiophene exhibits no changes in the UV-visible spectrum and only minimal changes in the voltammetric responses on exposure to Li⁺ or K⁺, there are large decreases in relative conductivities (69 and 47%, resp.). Thus, although the sensory properties of this polymer are expressed via several measurable entities, the ionoresistive response is clearly the most sensitive. This sensitivity originates from the cooperative nature of carrier transport in a conducting polymers (CP) and is thus inherent in chemoresistive CPs.

IT 171085-61-3P, 3,3'-Bis(2-hydroxyethoxy)-2,2'-bithiophene
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and NMR spectra of polythiophene receptors)

RN 171085-61-3 HCAPLUS

CN Ethanol, 2,2'-[[2,2'-bithiophene]-3,3'-diylbis(oxy)]bis- (9CI) (CA INDEX NAME)



L71 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:699277 HCAPLUS

DOCUMENT NUMBER: 123:83040

TITLE: Synthesis and Energy Transfer Properties of Terminally Substituted Oligothiophenes

AUTHOR(S): Wuerthner, Frank; Vollmer, Martin Siegfried; Effenberger, Franz; Emele, Peter; Meyer, Dirk Uwe; Port, Helmut; Wolf, Hans Christoph

CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Stuttgart, Stuttgart, D-70569, Germany

SOURCE: Journal of the American Chemical Society (1995), 117(31), 8090-9

PUBLISHER: CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: American Chemical Society

LANGUAGE: Journal

English

AB A series of conjugated anthryl-oligothienyl-porphyrins in which the oligothiophene is terminally linked to the 5-position of a porphyrin and to the 9-position of anthracene has been synthesized, and photoexcited-state properties have been studied by steady-state fluorescence spectra, fluorescence excitation spectra and picosecond time-resolved fluorescence measurements. Due to the spectral position of the anthracene and the porphyrin absorption bands a selective excitation of both end groups is possible, which is demonstrated by the UV-visible absorption spectra. Selective excitation of the anthryl end group leads to a quant. intramol. energy transfer to the porphyrin end

group in the subpicosecond time scale. The mechanism is discussed in terms of existing theories (Forster/Dexter, superexchange, and intramol. relaxation).

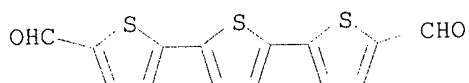
IT 13130-50-2P 32364-72-0P, [2,2'-Bithiophene]-5,5'-dicarboxaldehyde

RL: BYP (Byproduct); PREP (Preparation)

(synthesis and energy transfer properties of anthryl-oligothienyl-porphyrins)

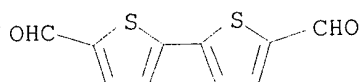
RN 13130-50-2 HCAPLUS

CN [2,2':5',2''-Terthiophene]-5,5''-dicarboxaldehyde (8CI, 9CI) (CA INDEX NAME)



RN 32364-72-0 HCAPLUS

CN [2,2'-Bithiophene]-5,5''-dicarboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



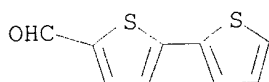
IT 3779-27-9, 5-Formyl-2,2'-bithiophene 7342-41-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis and energy transfer properties of anthryl-oligothienyl-porphyrins)

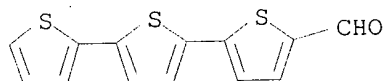
RN 3779-27-9 HCAPLUS

CN [2,2'-Bithiophene]-5-carboxaldehyde (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 7342-41-8 HCAPLUS

CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



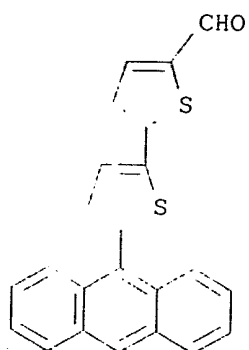
IT 165393-21-5P 165393-22-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

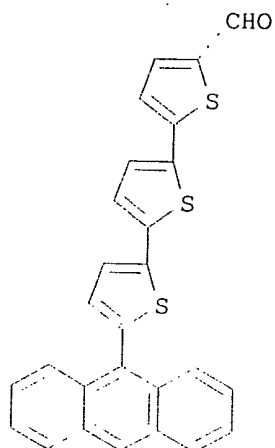
(synthesis and energy transfer properties of anthryl-oligothienyl-porphyrins)

RN 165393-21-5 HCAPLUS

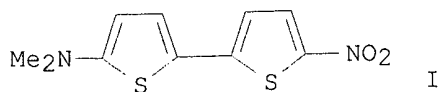
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-(9-anthracenyl)- (9CI) (CA INDEX NAME)



RN 165393-22-6 HCAPLUS
 CN [2,2':5',2''-Terthiophene]-5-carboxaldehyde, 5'-(9-anthracenyl)- (9CI)
 (CA INDEX NAME)



L71 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1995:466000 HCAPLUS
 DOCUMENT NUMBER: 123:32543
 TITLE: Synthesis and Solvatochromic Properties of
 Donor-Acceptor-Substituted Oligothiophenes
 AUTHOR(S): Effenberger, Franz; Wuerthner, Frank; Steybe, Felix
 CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet
 Stuttgart, Stuttgart, D-70569, Germany
 SOURCE: Journal of Organic Chemistry (1995), 60(7),
 2082-91
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



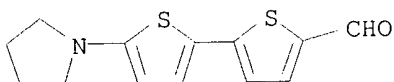
AB The Pd-catalyzed cross-coupling reaction of electron-donor-substituted thiophenes with electron-acceptor-substituted halothiophenes via organozinc intermediates or organotin compds. to give bi-, ter-, and quaterthiophenes is described. (Dimethylamino)bithiophenes with acceptor groups of varying reactivity were prepd. in 60-80% yield, whereas other bithiophenes were obtained as a mixt. with phenylthiophenes. Sym. substituted byproducts were formed in the conversion of 2-methoxythiophene with bromothiophenes via organozinc compds., yielding oligothiophenes. Ter- and quaterthiophenes were isolated in about 50-70% yield. The electronic interactions between donor and acceptor end groups in **conjugated** bithiophenes are expressed in the intense and markedly solvatochromic CT transitions. The solvatochromic behavior was detd. by linear regression analyses of absorption maxima in 11 solvents, whereby bithiophene I was found to be a very appropriate indicator dye, whose absorption wavenumbers in aliph. and dipolar aprotic solvents and, on consideration of the polarizability correction term $d.\delta.$, in arom. and chlorinated solvents excellently correlate with π^* values defined by Kamlet and Taft.

IT 146823-45-2P 149969-21-1P 150239-76-2P
150239-77-3P 163928-45-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and solvatochromism of donor-acceptor-substituted
oligothiophenes)

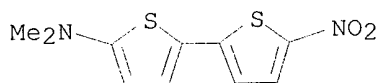
RN 146823-45-2 HCAPLUS

CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



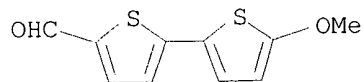
RN 149969-21-1 HCAPLUS

CN [2,2'-Bithiophen]-5-amine, N,N-dimethyl-5'-nitro- (9CI) (CA INDEX NAME)



RN 150239-76-2 HCAPLUS

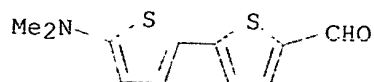
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-methoxy- (9CI) (CA INDEX NAME)



RN 150239-77-3 HCAPLUS

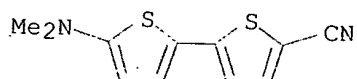
CN [2,2'-Bithiophene]-5-carboxaldehyde, 5'-(dimethylamino)- (9CI) (CA INDEX NAME)

NAME)



RN 163928-45-8 HCAPLUS

CN [2,2'-Bithiophene]-5-carbonitrile, 5'-(dimethylamino)- (9CI) (CA INDEX NAME)



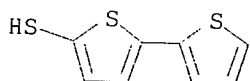
IT 159157-32-1, 5-Mercapto-2,2'-bithiophene

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. and solvatochromism of donor-acceptor-substituted oligothiophenes)

RN 159157-32-1 HCAPLUS

CN [2,2'-Bithiophene]-5-thiol (9CI) (CA INDEX NAME)



L71 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:314954 HCAPLUS

DOCUMENT NUMBER: 122:132487

TITLE: Quadratic nonlinear optical properties of some donor-acceptor substituted thiophenes

AUTHOR(S): Hutchings, Michael G.; Ferguson, Ian; McGeein, David J.; Morley, John O.; Zyss, Joseph; Ledoux, Isabelle

CORPORATE SOURCE: Zeneca Spec. Res. Cent., Blackey, M9 8ZS, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1995), (1), 171-6

CODEN: JCPKBH; ISSN: 0300-9580

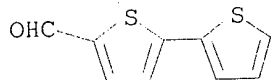
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

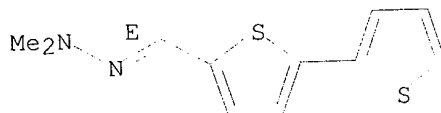
AB A series of thiophenes and bithiophenes contg. combinations of dimethylamino and dimethyl-hydrazono .pi.-acceptor groups was synthesized in order to study their non-linear optical properties. Soln. mol. hyperpolarizabilities were detd. by a combination of exptl. dipole moments and results from the elec. field induced second harmonic generation expt. Values obtained correlate well with those calcd. by the CNDOVSB MO method. The main structure-property relationships deduced from the results are: (i) thiophene provides a more efficient electron delocalization pathway than benzene; (ii) this increase is proportionately even greater for bithiophene compared with biphenyl; (iii) dimethylhydrazono results in twice the hyperpolarizability of dimethylamino in a comparable mol.; and (i.v.) dicyanovinyl is a more effective electron acceptor group than nitro in the thiophenes synthesized and calcd.

IT 3779-27-9P, [2,2'-Bithiophene]-5-carboxaldehyde
 160893-19-6P 160893-20-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (conversion to donor-acceptor substituted thiophenes with quadratic
 nonlinear optical properties)
 RN 3779-27-9 HCAPLUS
 CN [2,2'-Bithiophene]-5-carboxaldehyde (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



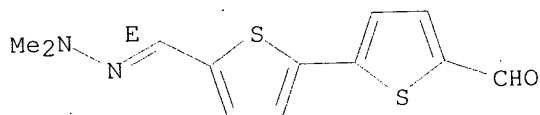
RN 160893-19-6 HCAPLUS
 CN [2,2'-Bithiophene]-5-carboxaldehyde, dimethylhydrazone, (E)- (9CI) (CA
 INDEX NAME)

Double bond geometry as shown.



RN 160893-20-9 HCAPLUS
 CN [2,2'-Bithiophene]-5,5'-dicarboxaldehyde, mono(dimethylhydrazone), (E)-
 (9CI) (CA INDEX NAME)

Double bond geometry as shown.



TRAN 09/871,353

see the d que for L57
for explanation of
this d que

=> d que 176

L1 19 SEA FILE=HCAPLUS ABB=ON PLU=ON CIPRIANI F?/AU
L2 135 SEA FILE=HCAPLUS ABB=ON PLU=ON GIGLI G?/AU
L3 377 SEA FILE=HCAPLUS ABB=ON PLU=ON CINGOLANI R?/AU
L4 48 SEA FILE=HCAPLUS ABB=ON PLU=ON FAVARETTO L?/AU
L5 59 SEA FILE=HCAPLUS ABB=ON PLU=ON ZAMBIANCHI M?/AU
L6 78 SEA FILE=HCAPLUS ABB=ON PLU=ON SOTGIU G?/AU
L7 71 SEA FILE=HCAPLUS ABB=ON PLU=ON CITRO G?/AU
L8 132 SEA FILE=HCAPLUS ABB=ON PLU=ON BARBARELLA G?/AU
L9 734 SEA FILE=HCAPLUS ABB=ON PLU=ON (L1 OR L2 OR L3 OR L4 OR L5
OR L6 OR L7 OR L8)
L10 54 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 AND THIOPHENE
L11 30 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 AND OLIGOMER?
L12 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L11 AND (THIOPHENE OLIGOMER)/T
I
L13 24 SEA FILE=REGISTRY ABB=ON PLU=ON (376393-41-8/BI OR 376393-42-
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111372-97-5/BI OR 111744-23-1/BI OR 113386-74-6/BI OR 116159-99
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201604-98-0/BI OR 25233-34-5/BI OR 376393-45-2/BI OR 5632-29-1/
BI OR 67984-20-7/BI)
L14 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L12 AND L13
L15 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L12 OR L14
L16 STR₀

11
Q
||
||
Hy[^]Hy[^]Hy G1 4 Q[~]C A⁼⁼C Q⁼⁼C⁼⁼N
1 2 3 @5 @6 7 @8 9 10 @12

VAR G1=5/6/8/12/NH2/OH/SH/SO3H/SO2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

GGCAT IS MCY UNS AT 2

GGCAT IS MCY UNS AT 3

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E4 C E1 S AT 1

ECOUNT IS E4 C E1 S AT 2

ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L17 289013 SEA FILE=REGISTRY ABB=ON PLU=ON 16.145.3/RID
L19 STR

Hy[^]Hy[^]Hy
1 2 3

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 1

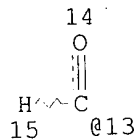
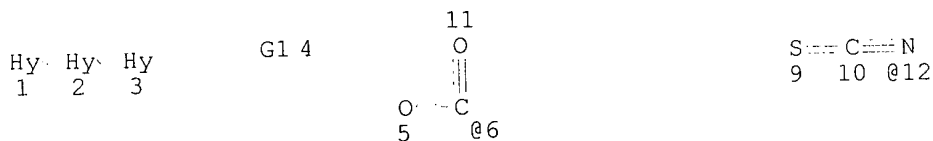
GGCAT IS MCY UNS AT 2

GGCAT IS MCY UNS AT 3

DEFAULT ECLEVEL IS LIMITED
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 ECOUNT IS E4 C E1 S AT 2
 ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE
 L21 5115 SEA FILE=REGISTRY SUB=L17 SSS FUL L19
 L23 2293 SEA FILE=REGISTRY SUB=L21 SSS FUL L16
 L26 STR



VAR G1=OH/SH/NH2/13/6/12

NODE ATTRIBUTES:
 CONNECT IS E1 RC AT 5
 DEFAULT MLEVEL IS ATOM
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 GGCAT IS MCY UNS AT 2
 GGCAT IS MCY UNS AT 3
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS E4 C E1 S AT 1
 ECOUNT IS E4 C E1 S AT 2
 ECOUNT IS E4 C E1 S AT 3

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
 L27 1357 SEA FILE=REGISTRY SUB=L23 SSS FUL L26
 L28 476 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 3 16.145.3/RID
 L29 166 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 4 16.145.3/RID
 L30 104 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND 5 16.145.3/RID
 L31 746 SEA FILE=REGISTRY ABB=ON PLU=ON (L28 OR L29 OR L30)
 L32 674 SEA FILE=REGISTRY ABB=ON PLU=ON L31 AND NC=1 NOT ("DIAZO" OR
 F/ELS)
 L72 6 SEA FILE=REGISTRY ABB=ON PLU=ON L32 AND "ISOTHIOCYANATO"
 L75 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L72
 L76 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L75 NOT L15

=> d ibib abs hitstr

L76 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:792698 HCAPLUS

DOCUMENT NUMBER: 136:66480

TITLE: Oligothiophene isothiocyanates as a new class of fluorescent markers for biopolymers

AUTHOR(S): Barbarella, Giovanna; Zambianchi, Massimo; Pudova, Olga; Paladini, Vanessa; Ventola, Alfredo; Cipriani, Francesco; Gigli, Giuseppe; Cingolani, Roberto; Citro, Gennaro

CORPORATE SOURCE: Consiglio Nazionale Ricerche, I.Co.C.E.A, Bologna, 40129, Italy

SOURCE: Journal of the American Chemical Society (2001), 123(47), 11600-11607

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The regioselective synthesis of fluorescent oligothiophene isothiocyanates is described. The isothiocyanates were reacted with bovine serum albumin (BSA) following std. procedures and the optical properties of the oligothiophene-BSA conjugates were analyzed as a function of oligomer concn., time, and irradiation power. The oligothiophene-BSA conjugates were chem. very stable and their photoluminescence characteristics persisted unaltered for several months. Photoluminescence data relative to the conjugate of an oligothiophene-S,S-dioxide isothiocyanate with monoclonal anti-CD8 antibody are reported. No fluorescence quenching was observed following the binding of the isothiocyanate to the antibody and the conjugate displayed high chem. stability and photostability.

IT 376393-41-8DP, reaction conjugated with bovine serum albumin

385369-25-5DP, reaction conjugated with bovine serum albumin

385369-31-3DP, reaction conjugated with bovine serum albumin

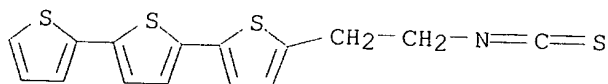
385369-34-6DP, reaction conjugated with CD8 antibody

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)

(oligothiophene isothiocyanates as a new class of fluorescent markers for biopolymers)

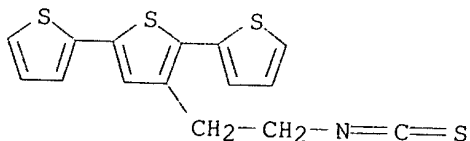
RN 376393-41-8 HCAPLUS

CN 2,2':5',2''-Terthiophene, 5-(2-isothiocyanatoethyl)- (9CI) (CA INDEX NAME)



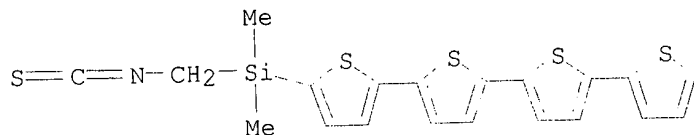
RN 385369-25-5 HCAPLUS

CN 2,2':5',2''-Terthiophene, 3'-(2-isothiocyanatoethyl)- (9CI) (CA INDEX NAME)

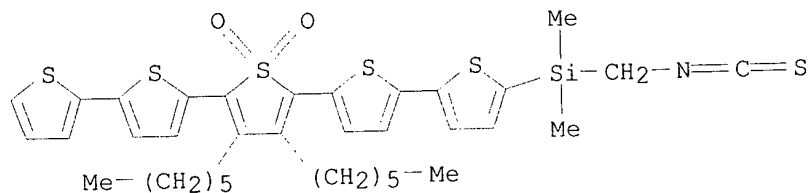


TRAN 09/871,353

RN 385369-31-3 HCAPLUS
CN Silane, (isothiocyanatomethyl)dimethyl[2,2':5',2'':5'',2''':5''',2''''-
quaterthiophen]-5-yl- (9CI) (CA INDEX NAME)



RN 385369-34-6 HCAPLUS
CN Silane, (3'',4''-dihexyl-1'',1''-dioxido[2,2',5':2'':5'',2''':5''',2''''-
quinguethiophen]-5-yl)(isothiocyanatomethyl)dimethyl- (9CI) (CA INDEX
NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT